

=> file caplus
COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
193.85	194.06

FULL ESTIMATED COST

FILE 'CAPLUS' ENTERED AT 14:30:22 ON 15 JUL 2007
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FILE COVERS 1907 - 15 Jul 2007 VOL 147 ISS 4
FILE LAST UPDATED: 13 Jul 2007 (20070713/ED)

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=> d 12
YOU HAVE REQUESTED DATA FROM FILE 'REGISTRY' - CONTINUE? (Y)/N:n

=> s 12
L3 14 L2

=> d 13 1-14 ibib abs

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9
exact/norm bonds :
5-7 6-9 7-8 7-13 8-9 10-11 10-12 13-14
exact bonds :
8-10
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6

G1:Cb,Ak

Match level :

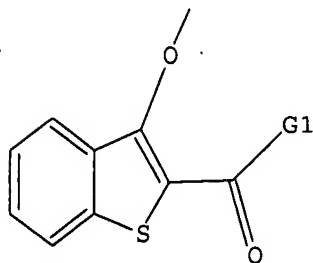
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:CLASS

L1 STRUCTURE UPLOADED

=> d

L1 HAS NO ANSWERS

L1 STR



G1 Cb,Ak

Structure attributes must be viewed using STN Express query preparation.

=> s l1 full

FULL SEARCH INITIATED 14:28:59 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 1902 TO ITERATE

100.0% PROCESSED 1902 ITERATIONS

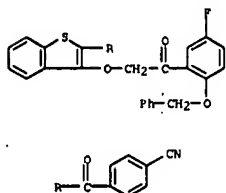
169 ANSWERS

SEARCH TIME: 00.00.01

L2 169 SEA SSS FUL L1

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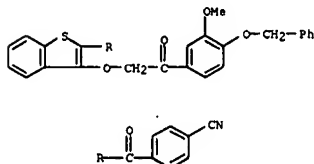
L2 ANSWER 1 OF 169 REGISTRY COPYRIGHT 2007 ACS on STN
 RN 852430-73-0 REGISTRY
 ED Entered STN: 16 Jun 2005
 CN Benzonitrile, 4-[[3-[2-[5-fluoro-2-(phenylmethoxy)phenyl]-2-oxoethoxy]benzo[b]thien-2-yl]carbonyl]- (9CI) (CA INDEX NAME)
 OTHER NAMES:
 CN 4-[[3-[2-(2-Benzylloxy-5-fluorophenyl)-2-oxoethoxy]benzo[b]thien-2-yl]carbonyl]benzonitrile
 MF C31 H20 F N O4 S
 SR CA
 LC STN Files: CA, CAPLUS, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

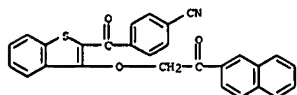
L2 ANSWER 2 OF 169 REGISTRY COPYRIGHT 2007 ACS on STN
 RN 852430-72-9 REGISTRY
 ED Entered STN: 16 Jun 2005
 CN Benzonitrile, 4-[[3-[2-[3-methoxy-4-(phenylmethoxy)phenyl]-2-oxoethoxy]benzo[b]thien-2-yl]carbonyl]- (9CI) (CA INDEX NAME)
 OTHER NAMES:
 CN 4-[[3-[2-(4-Benzylloxy-3-methoxyphenyl)-2-oxoethoxy]benzo[b]thien-2-yl]carbonyl]benzonitrile
 MF C32 H23 N O5 S
 SR CA
 LC STN Files: CA, CAPLUS, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

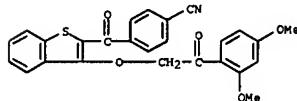
L2 ANSWER 3 OF 169 REGISTRY COPYRIGHT 2007 ACS on STN
 RN 852430-71-8 REGISTRY
 ED Entered STN: 16 Jun 2005
 CN Benzonitrile, 4-[[3-[2-(2-naphthalenyl)-2-oxoethoxy]benzo[b]thien-2-yl]carbonyl]- (9CI) (CA INDEX NAME)
 OTHER NAMES:
 CN 4-[[3-[2-(Naphthalen-2-yl)-2-oxoethoxy]benzo[b]thien-2-yl]carbonyl]benzonitrile
 MF C28 H17 N O3 S
 SR CA
 LC STN Files: CA, CAPLUS, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

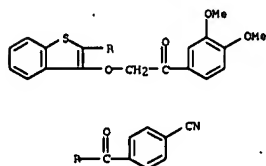
L2 ANSWER 4 OF 169 REGISTRY COPYRIGHT 2007 ACS on STN
 RN 852430-70-7 REGISTRY
 ED Entered STN: 16 Jun 2005
 CN Benzonitrile, 4-[[3-[2-(2,4-dimethoxyphenyl)-2-oxoethoxy]benzo[b]thien-2-yl]carbonyl]- (9CI) (CA INDEX NAME)
 OTHER NAMES:
 CN 4-[[3-[2-(2,4-Dimethoxyphenyl)-2-oxoethoxy]benzo[b]thien-2-yl]carbonyl]benzonitrile
 MF C26 H19 N O5 S
 SR CA
 LC STN Files: CA, CAPLUS, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

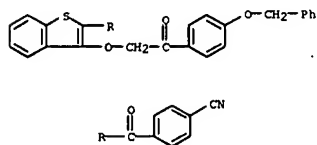
L2 ANSWER 5 OF 169 REGISTRY COPYRIGHT 2007 ACS on STN
 RN 852430-69-4 REGISTRY
 ED Entered STN: 16 Jun 2005
 CN Benzonitrile, 4-[[3-[2-(3,4-dimethoxyphenyl)-2-oxoethoxy]benzo[b]thien-2-yl]carbonyl]- (9CI) (CA INDEX NAME)
 OTHER NAMES:
 CN 4-[[3-[2-(3,4-Dimethoxyphenyl)-2-oxoethoxy]benzo[b]thien-2-yl]carbonyl]benzonitrile
 MF C26 H19 N O5 S
 SR CA
 LC STN Files: CA, CAPLUS, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

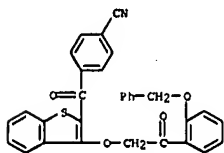
L2 ANSWER 6 OF 169 REGISTRY COPYRIGHT 2007 ACS on STN
 RN 852430-68-3 REGISTRY
 ED Entered STN: 16 Jun 2005
 CN Benzonitrile, 4-[[3-[2-oxo-2-(4-(phenylmethoxy)phenyl)ethoxy]benzo[b]thien-2-yl]carbonyl]- (9CI) (CA INDEX NAME)
 OTHER NAMES:
 CN 4-[[3-[2-(4-Benzoyloxyphenyl)-2-oxoethoxy]benzo[b]thien-2-yl]carbonyl]benzonitrile
 MF C31 H21 N O4 S
 SR CA
 LC STN Files: CA, CAPLUS, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

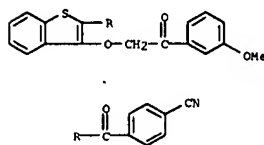
L2 ANSWER 7 OF 169 REGISTRY COPYRIGHT 2007 ACS on STN
 RN 852430-67-2 REGISTRY
 ED Entered STN: 16 Jun 2005
 CN Benzonitrile, 4-[[3-[2-oxo-2-(2-(phenylmethoxy)phenyl)ethoxy]benzo[b]thien-2-yl]carbonyl]- (9CI) (CA INDEX NAME)
 OTHER NAMES:
 CN 4-[[3-[2-(2-Benzoyloxyphenyl)-2-oxoethoxy]benzo[b]thien-2-yl]carbonyl]benzonitrile
 MF C31 H21 N O4 S
 SR CA
 LC STN Files: CA, CAPLUS, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

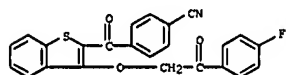
L2 ANSWER 8 OF 169 REGISTRY COPYRIGHT 2007 ACS on STN
 RN 852430-66-1 REGISTRY
 ED Entered STN: 16 Jun 2005
 CN Benzonitrile, 4-[[3-[2-(3-methoxyphenyl)-2-oxoethoxy]benzo[b]thien-2-yl]carbonyl]- (9CI) (CA INDEX NAME)
 OTHER NAMES:
 CN 4-[[3-[2-(3-Methoxyphenyl)-2-oxoethoxy]benzo[b]thien-2-yl]carbonyl]benzonitrile
 MF C25 H17 N O4 S
 SR CA
 LC STN Files: CA, CAPLUS, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

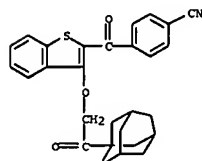
L2 ANSWER 9 OF 169 REGISTRY COPYRIGHT 2007 ACS on STN
 RN 852430-65-0 REGISTRY
 ED Entered STN: 16 Jun 2005
 CN Benzonitrile, 4-[[3-[2-(4-fluorophenyl)-2-oxoethoxy]benzo[b]thien-2-yl]carbonyl]- (9CI) (CA INDEX NAME)
 OTHER NAMES:
 CN 4-[[3-[2-(4-Fluorophenyl)-2-oxoethoxy]benzo[b]thien-2-yl]carbonyl]benzonitrile
 MF C24 H14 F N O3 S
 SR CA
 LC STN Files: CA, CAPLUS, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L2 ANSWER 10 OF 169 REGISTRY COPYRIGHT 2007 ACS on STN
 RN 852430-64-9 REGISTRY
 ED Entered STN: 16 Jun 2005
 CN Benzonitrile, 4-[[3-(2-oxo-2-tricyclo[3.3.1.1^{3,7}]dec-1-ylethoxy)benzo[b]thien-2-yl]carbonyl]- (9CI) (CA INDEX NAME)
 OTHER NAMES:
 CN 4-[[3-[2-(Adamantan-1-yl)-2-oxoethoxy]benzo[b]thien-2-yl]carbonyl]benzonitrile
 MF C28 H25 N O3 S
 SR CA
 LC STN Files: CA, CAPLUS, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

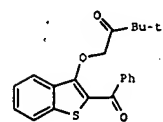
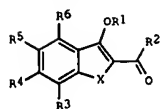
1 REFERENCES IN FILE CA (1907 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L3 ANSWER 1 OF 14 CAPLUS COPYRIGHT 2007 ACS ON STN

ACCESSION NUMBER: 20051453342 CAPLUS
DOCUMENT NUMBER: 143:7588
TITLE: Preparation of benzofuran and benzothiophene derivatives as antidiabetic agents
INVENTOR(S): Molinet, Gerard; Leriche, Caroline; Kergoat, Micheline
PATENT ASSIGNER(S): Merck Santé, Fr.
SOURCE: Fr. Demande, 55 pp.
CODEN: FXXXDL
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2862646	A1	20050527	FR 2003-13615	20031120
FR 2862646	B1	20060224		
AU 2004295036	A1	20050616	AU 2004-295036	20041108
CA 2546651	A1	20050616	CA 2004-2546651	20041108
WO 2005054226	A1	20050616	WO 2004-EP12620	20041108
W: AR, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SN, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BV, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1685122	A1	20060802	EP 2004-797711	20041108
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK, IS				
CN 1882562	A	20061220	CN 2004-80034191	20041108
BR 2004016790	A	20070306	BR 2004-16790	20041108
JP 2007511556	T	20070510	JP 2006-540238	20041108
IN 2006KN00984	A	20070420	IN 2006-KN984	20060419
US 2007066680	A1	20070322	US 2006-579996	20060519
PRIORITY APPLN. INFO.:			FR 2003-13615	A 20031120
OTHER SOURCE(S):			WO 2004-EP12620	W 20041108
GI			CASREACT 143:7588; MARPAT 143:7588	

L3 ANSWER 1 OF 14 CAPLUS COPYRIGHT 2007 ACS ON STN (Continued)



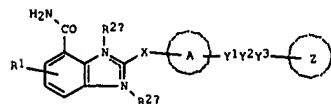
AB Title compds. I [wherein X = O, S; R1 = carbonylalkyl, alkoxyalkyl, arylalkyl, alkyl, etc.; R2 = cycloalkyl, aryl; R3, R4, R5, R6 = independently H, halo, OH, alkyl, alkoxy, CN, CF3, NO2, NH2 and derivs.; their stereoisomers, racemates and pharmaceutically acceptable salts] were prepared as antidiabetic agents for treat diseases associated with insulin resistance syndrome. For example, II was prepared by cyclocondensation of thiosalicylic acid with 2-bromoacetophenone, followed by reaction with 1-bromopinacolone. In an in vitro test, at 10⁻⁶ M, II displayed a glucose-induced stimulation factor of insulin secretion of 183% at a dose of 8 mM glucose digested by the pancreatic exocrine tissue of rats. II, when administered orally to NOD2 rats, reduced glycemia level by 23%. Thus, and their compns. are used for treating hyperglycemia, diabetes, dyslipidemia, obesity, and microvascular and macrovascular complications arising from diabetes.

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 2 OF 14 CAPLUS COPYRIGHT 2007 ACS ON STN

ACCESSION NUMBER: 2002:676008 CAPLUS
DOCUMENT NUMBER: 137:216949
TITLE: Preparation of benzimidazole derivatives as poly(ADP-ribose) polymerase (PARP) inhibitors
INVENTOR(S): Takayama, Kazuhisa; Kimura, Takenori; Masuda, Naoyuki; Naito, Ryo; Okamoto, Yoshinori; Koga, Yuji; Okada, Yohel; Takeuchi, Makoto
PATENT ASSIGNER(S): Yamanouchi Pharmaceutical Co., Ltd., Japan
SOURCE: PCT Int. Appl., 46 pp.
CODEN: PXXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002068407	A1	20020906	WO 2002-JP1741	20020226
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2002233746	A1	20020912	AU 2002-233746	20020226
PRIORITY APPLN. INFO.:			JP 2001-54693	A 20010228
OTHER SOURCE(S):			WO 2002-JP1741	W 20020226
GI			MARPAT 137:216949	



AB The title compds. I [R1 = H, alkyl, etc.; R2a, R2b = H, alkyl, or nonexistent; the dotted line indicates the double bond or single bond; ring A = N-containing saturated heterocyclic ring; X = (oxo-substituted) alkylene, or bond; Y1, Y3 = (oxo-substituted) alkylene, etc.; Y2 = O, S, etc.; ring Z = (un)substituted cycloalkyl, etc.; provisos are given] are prepared 2-[1-[4-(4-fluorophenyl)butyl]piperidin-4-yl]-1H-benzimidazole-4-carboxamide 2HCl salt in vitro showed IC50 of 8.2 nM against poly(ADP-ribose) polymerase.

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

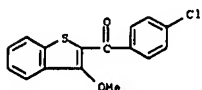
L3 ANSWER 3 OF 14 CAPLUS COPYRIGHT 2007 ACS ON STN

ACCESSION NUMBER: 1998:757786 CAPLUS
DOCUMENT NUMBER: 130:95444
TITLE: Synthesis of (4-chlorophenyl)-(1-oxo-1,4-benzo[b]thien-2-yl)methanone and study of its reactivity towards sulfur- and oxygen-containing nucleophiles
AUTHOR(S): Pouzet, Pascale; Erdelmeier, Irene; Dansette, Patrick M.; Mansuy, Daniel
CORPORATE SOURCE: Laboratoire de Chimie et Biochimie Pharmacologiques et Toxicologiques (URA 400), Université René Descartes, Paris, 75270, Fr.
SOURCE: Tetrahedron (1998), 54(49), 14811-14824
CODEN: TETRAH; ISSN: 0040-4020
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 130:95444

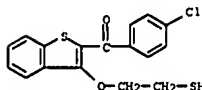
AB (4-Chlorophenyl)-(1-oxo-1,4-benzo[b]thien-2-yl)methanone was synthesized by oxidation of the corresponding benzo[b]thiophene derivative with the oxidative system H2O2/TFA. This benzo[b]thiophene sulfone undergoes Michael-type nucleophilic addition of sulfur- and oxygen-containing nucleophiles either under basic conditions leading to 3-substituted 2,3-dihydrobenzo[b]thiophene 1-oxides or in acidic media leading then to re-aromatized 3-substituted benzo[b]thiophenes. This method provides an easy two-step functionalization of 2-acylbenzo[b]thiophene derivatives.

REFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ACCESSION NUMBER: 1998:757786 CAPLUS
 DOCUMENT NUMBER: 130:95444
 TITLE: Synthesis of (4-chlorophenyl)-(1-oxo-1,4-benzo[b]thien-2-yl)methanone and study of its reactivity towards sulfur- and oxygen-containing nucleophiles
 AUTHOR(S): Pouzet, Pascale; Erdelmeier, Irene; Danzette, Patrick M.; Mansuy, Daniel
 CORPORATE SOURCE: Laboratoire de Chimie et Biochimie Pharmacologiques et Toxicologiques (URA 400), Université René Descartes, Paris, 75270, Fr.
 SOURCE: Tetrahedron (1998), 54(49), 14811-14824
 CODEN: TETRA8; ISSN: 0040-4020
 PUBLISHER: Elsevier Science Ltd.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 130:95444
 AB (4-Chlorophenyl)-(1-oxo-1,4-benzo[b]thien-2-yl)methanone was synthesized by oxidation of the corresponding benzo[b]thiophene derivative with the oxidative system H₂O₂/TFA. This benzo[b]thiophene sulfoxide undergoes Michael-type nucleophilic addition of sulfur- and oxygen-containing nucleophiles either under basic conditions leading to 3-substituted 2,3-dihydrobenzo[b]thiophene 1-oxides or in acidic media leading then to re-aromatized 3-substituted benzo[b]thiophenes. This method provides an easy two-step functionalization of 2-acylbenzo[b]thiophene derivs.
 IT 219506-10-2P 219506-28-2P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of (chlorophenyl)oxobenzothiénylmethanone and its reactions with sulfur- and oxygen-containing nucleophiles)
 RN 219506-10-2 CAPLUS
 CN Methanone, (4-chlorophenyl) (3-methoxybenzo[b]thien-2-yl)- (SCI) (CA INDEX NAME)



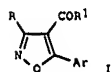
RN 219506-28-2 CAPLUS
 CN Methanone, (4-chlorophenyl) [3-(2-mercaptoethoxy)benzo[b]thien-2-yl]- (SCI)
 (CA INDEX NAME)



REFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

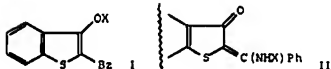
ACCESSION NUMBER: 1995:995026 CAPLUS
 DOCUMENT NUMBER: 124:117307
 TITLE: Preparation of isoxazole derivatives as herbicides
 INVENTOR(S): Geach, Neil; Hawkins, David William; Pearson, Christopher John; Smith, Philip Henry Gaunt; White, Nicolas
 PATENT ASSIGNEE(S): Rhone-Poulenc Agriculture Ltd., UK
 SOURCE: PCT Int. Appl., 44 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9525105	A1	19950921	WO 1995-EP951	19950314
V: AM, AU, BB, EG, BR, BY, CA, CN, CZ, EE, FI, GE, HU, KG, KP, KR, KZ, LX, LR, LT, LV, MD, MG, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TJ, TT, UA, UG, US, UZ, VN				
RW: KE, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9518943	A	19951003	AU 1995-18943	19950314
PRIORITY APPLN. INFO.: GB 1994-5234 A 19940317				
WO 1995-EP951 W 19950314				
OTHER SOURCE(S): MARPAT 124:117307				
GI				



AB The title isoxazoles I [Ar represents a monocyclic or fused bicyclic heterocyclic system Het having a non-pyridyl heterocyclic first ring and an optional second heterocyclic or carbocyclic ring, the second ring when present being fused to the first ring, the first ring having from 1 to 4 hetero ring atoms and from 4 to 7 total ring atoms, the first ring being aromatic or non-aromatic and being optionally substituted by from 1 to 4 R2 groups which may be the same or different, the second ring being optionally substituted by from 1 to 4 R2 groups which may be the same or different; R represents the hydrogen atom or a group CO2R3; R1 represents a straight- or branched-chain alkyl group containing from one to six carbon atoms which is optionally substituted by one or more halogen atoms; or a cycloalkyl group containing from three to six carbon atoms optionally substituted by one or more groups selected from R4, CO2R4, SR4, halogen and OR4; R2 represents a halogen atom, a straight- or branched-chain alkyl group containing from one to six carbon atoms which is substituted by a group OR4; or a group selected from OH, R4, etc.; a proviso is given; R3 and R4 each represents alkyl, alkenyl, etc.] are claimed. 4-Cyclopropylcarbonyl-5-(2,2-difluoro-1,3-benzodioxol-4-yl)isoxazole (preparation given) at 4 Kg/ha pre- or post-emergence gave 90% control of one or more weed species (Abutilon theophrasti, Avena fatua, etc.).

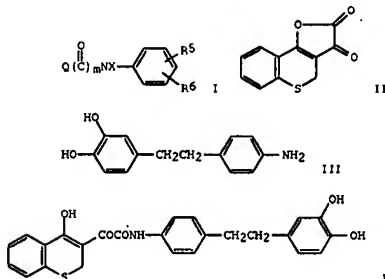
ACCESSION NUMBER: 1988:221534 CAPLUS
 DOCUMENT NUMBER: 108:221534
 TITLE: Benzo-quinoid tautomerism of azomethines and their structural analogs. 15. Synthesis and properties of 2-(aminobenzylidene)-3-(2H)-benzo[b]thiophene derivatives
 AUTHOR(S): Shepelenko, E. N.; Bren, V. A.; Andreichikova, G. E.
 CORPORATE SOURCE: Inst. Fiz. Org. Khim., Rostov, USSR
 SOURCE: Khimiya Geterotsiklicheskih Soedinenii (1987), (8), 1043-6
 CODEN: KOSSAQ; ISSN: 0453-8234
 DOCUMENT TYPE: Journal
 LANGUAGE: Russian
 OTHER SOURCE(S): CASREACT 108:221534
 GI



AB A series of 2-benzoyl-3-acyloxybenzo[b]thiophenones I (X = H, Ac), 2-[N-aryl(alkyl)aminobenzylidene]-3(2H)-benzo[b]thiophenones II (X = H, Ac), and their N-formyl derivs., having a tautomeric aminobenzylidene ketone structure, were prepared and their structures were confirmed by UV, IR, and NMR spectra.

ACCESSION NUMBER: 1988:21703 CAPLUS
 DOCUMENT NUMBER: 108:21703
 TITLE: Preparation of heterocyclic enol amide derivatives as pharmaceuticals
 PATENT ASSIGNEE(S): Warner-Lambert Co., USA
 SOURCE: Jpn. Kokai Tokkyo Koho, 78 pp.
 CODEN: JKKXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 62081369	A	19870414	JP 1986-230231	19860930
US 4761424	A	19880802	US 1985-782623	19851001
ZA 8606973	A	19880427	ZA 1986-6973	19860912
AU 8663285	A	19870402	AU 1986-63285	19860929
AU 605747	B2	19910124		
DK 8604664	A	19870406	DK 1986-4664	19860930
EP 221345	A1	19870513	EP 1986-113489	19861001
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
ES 2002398	A6	19880801	ES 1986-2338	19861001
US 4921871	A	19900501	US 1987-121264	19871116
US 4874758	A	19891017	US 1988-164355	19880304
US 4868195	A	19890919	US 1988-165045	19880307
US 4868200	A	19890919	US 1988-166146	19880309
US 4868199	A	19890919	US 1988-167264	19880309
US 4868205	A	19890919	US 1988-167272	19880311
PRIORITY APPLN. INFO.: US 1985-782623 A 19851001				
US 1987-121264 A3 19871116				
OTHER SOURCE(S): CASREACT 108:21703; MARPAT 108:21703				
GI				

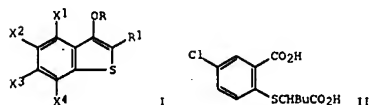


AB The title compds. (I; Q = benzofuryl, benzothienyl, indolyl, benzopyranyl, benzothienopyranyl, etc.; R5 = H, C1-4 alkyl, alkoxy, C2-4 carbalkoxy, etc.)

L3 ANSWER 6 OF 14 CAPLUS COPYRIGHT 2007 ACS ON STN (Continued)
 R6 = C6-20 alkyl, styryl, etc.; X = H, alkyl; m = 1, 2), useful as pharmaceuticals, are prepd. A mixt. of 0.085 mol furandione deriv. II and 0.0749 mol aniline deriv. III in THF was stirred at room temp. under N, the solvent distd. in vacuo, and the solid product was refluxed in CH₂Cl₂ to give 85.2% enol amide IV. I showed ID50 against 5-lipoxygenase at 1.06-9.30M.

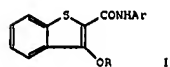
L3 ANSWER 7 OF 14 CAPLUS COPYRIGHT 2007 ACS ON STN
 ACCESSION NUMBER: 1987:515480 CAPLUS
 DOCUMENT NUMBER: 107:115480
 TITLE: Preparation of benzo[b]thiophenes as arachidonate oxidation inhibitors
 INVENTOR(S): Durette, Philippe L.; Witzel, Bruce E.; Rupprecht, Kathleen M.; Tischler, Allan N.; Gallagher, Timothy F.
 PATENT ASSIGNEE(S): Merck and Co., Inc., USA
 SOURCE: S. African, 78 pp.
 CODEN: SFXKAB
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
ZA 8661709	A	19861029	ZA 1986-1709	19860307
US 4663344	A	19870505	US 1985-710727	19850311
PRIORITY APPLN. INFO.:		US 1985-710727 A 19850311		
OTHER SOURCE(S):		CASREACT 107:115480; MARPAT 107:115480		
GI				



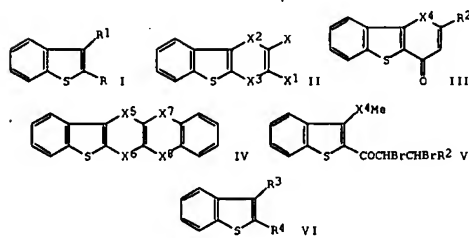
AB The title compds. [I; R = H, acyl, cycloalkyl, (un)substituted alkyl, (un)modified CO₂H, etc.; R1 = H, aryl, cycloalkyl, (un)substituted alkyl, alkenyl, alkynyl, Ph, PhCH₂, heteroaryl; X1-X4 = H, alkenyl, naphthyl, alkoxy, alkylthio, acyl, amino, cyano, halo, OH, SH, NO, NO₂, (un)substituted alkyl, Ph, imidazol-2-yl] were prepared as arachidonate oxidation inhibitors. 5,2-Cl(HS)C₆H₃CO₂H was refluxed with BuCHBrCO₂H in aqueous NaOH to give [(carboxyphenyl)thio]hexanoate II. II was heated with NaOAc and Ac₂O to give 40% overall I (R = Ac, R1 = Bu, X1 = X3 = X4 = H, X2 = Cl), which gave >95% inhibition of RBL cell 5-lipoxygenase at 15 μM.

L3 ANSWER 8 OF 14 CAPLUS COPYRIGHT 2007 ACS ON STN
 ACCESSION NUMBER: 1985:466721 CAPLUS
 DOCUMENT NUMBER: 103:66721
 TITLE: Activities of 2-carboxanilido-3-hydroxybenzo[b]thiophenes against the mollusk Biomphalaria glabrata
 AUTHOR(S): Gayral, Philippe; Bulsion, Jean Pierre; Royer, Rene
 CORPORATE SOURCE: Fac. Pharm., Univ. Paris-Sud, Chateau-Malabry, 92290, Fr.
 SOURCE: European Journal of Medicinal Chemistry (1985), 20(2), 187-9
 CODEN: EJMCA5; ISSN: 0223-5234
 DOCUMENT TYPE: Journal
 LANGUAGE: French
 OTHER SOURCE(S): CASREACT 103:66721
 GI



AB 2-Carboxanilido-3-hydroxybenzo[b]thiophenes I (R = H or Ac, Ar = Ph or substituted Ph), prepared by the condensation of thioalicyclic acid [147-93-3] with substituted chloroacetanilides, in DMF, in presence of NaOAc, have molluscicidal activity, which is structure-dependent. Hydroxylated amide deriva. of I are active against Biomphalaria glabrata, at 1 and 10 mg/L, and have activities almost as high as Niclosamide. The replacement of OH by Ac had no effect on activity. Data of the activity of 37 compds. examined indicated that the molluscicidal activity is determined by the benzamidic moiety. Compds. such as I[R = H, Ar = C₆H₃(NO₂)OMe-2,4] [97457-75-5], I[R = H, Ar = C₆H₃Cl(NO₂)-2,4] [97457-76-6], and I[R = H, Ar = C₆HCl₄-2,3,5,6] [97457-77-7] were completely inactive.

L3 ANSWER 9 OF 14 CAPLUS COPYRIGHT 2007 ACS ON STN
 ACCESSION NUMBER: 1978:443182 CAPLUS
 DOCUMENT NUMBER: 89:43182
 TITLE: Synthesis of flavones and xanthenes in the benzo[4,5]thiophene series
 AUTHOR(S): Netchitailo, P.; Decroix, Bernard; Morel, Jean; Pastour, Paul
 CORPORATE SOURCE: Lab. Chim. Org. Heterocyclique, Inst. Sci. Haute-Normandie, Mont-Saint-Aignan, Fr.
 SOURCE: Journal of Heterocyclic Chemistry (1978), 15(2), 337-42
 CODEN: JHTCAD; ISSN: 0022-152X
 DOCUMENT TYPE: Journal
 LANGUAGE: French
 OTHER SOURCE(S): CASREACT 89:43182
 GI



AB 2-[3-(3-methoxybenzothienyl)thio]benzo[b]thiophene condensed with 3-methoxy-2-thiophenecarbonyl chloride or o-MeOC₆H₄COCl to give the corresponding acylmethoxybenzothienopyranones I (R = H, R1 = 3-methoxy-2-thienylcarbonyl, o-MeOC₆H₄CO, and vice versa), which cyclized in HCl-pyridine to give the benzothienopyranones II [XXI = CH:CHCH:CH, CH:CHS, SCH:CH; X2, X3 = O, CO, but X2 ≠ X3]. The benzothienopyranones and -thiopyranones (III, R2 = Ph, C₆H₄OMe-p; X4 = O, S) and the bis(benzothienopyranones (IV, X5, X6 = O or CO, but X5 ≠ X6; X7, X8 = - or S but X7 ≠ X8) were prepared by cyclizing V or VI (R3 = OMe, R4 = 3-methoxybenzothien-2-ylcarbonyl or vice versa; resp.).

L3 ANSWER 10 OF 14 CAPLUS COPYRIGHT 2007 ACS ON STN
ACCESSION NUMBER: 1970:121469 CAPLUS
DOCUMENT NUMBER: 72:121469
TITLE: Rearrangement of benzothiazine sulfoxides
AUTHOR(S): Morin, Robert B.; Spry, Douglas O.
CORPORATE SOURCE: Lilly Res. Lab., Eli Lilly and Co., Indianapolis, IN, USA
SOURCE: Journal of the Chemical Society [Section] D: Chemical Communications (1970), (6), 335-6
CODEN: CCJDAO; ISSN: 0577-6171
JOURNAL

DOCUMENT TYPE:
LANGUAGE: English

G1 For diagram(s), see printed CA Issue.

AB Reaction of substituted benzothiazine sulfoxides with Ac2O under reflux leads by an elimination reaction to a sulfenic acid derivative that undergoes subsequent addition to the double bond formed if the N is tertiary but is trapped as a cyclic sulfenamide by a secondary N. Oxidizing I (R = H) with m-ClC6H4CO2OH (II) in CHCl3 at -5° gave the sulfoxide, m. 128-9°, which was refluxed with Ac2O containing 1% NaOAc to give a 3:2 mixture of III (R = OMe;CH2) (III), presumably via IV, and V (R = H). Refluxing the sulfoxide of I (R = Me), m. 80-2°, with Ac2O-NaOAc gave 50% VI (R = C(OAc);CH2) (VII), variable yields of the interconvertible VI (R = H) and VIII (neither of which gave VII under the reaction conditions), and approx. 10% V (R = Ac), all via IV (R = Me) (IX). Acetylation of the enamide IX followed by addition of the sulfenic group to the substituted double bond and enol acetylation presumably gave VII. The sole oxidation product from X by oxidation with II at room temperature of using O3 at -70° was III (R = Me), apparently via the sulfoxide followed by elimination; the generated sulfenic acid reacts with the neighboring amide group.

L3 ANSWER 11 OF 14 CAPLUS COPYRIGHT 2007 ACS ON STN
ACCESSION NUMBER: 1968:467165 CAPLUS
DOCUMENT NUMBER: 69:67165
TITLE: Syntheses of 2-methoxy- and 3-methoxythianaphthenes
AUTHOR(S): Matsuki, Yasuo; Adachi, Yoshio
CORPORATE SOURCE: Tohoku Univ., Sendai, Japan
SOURCE: Nippon Kagaku Zasshi (1968), 89(2), 192-6
CODEN: NPKZAZ; ISSN: 0369-5387
JOURNAL

DOCUMENT TYPE:
LANGUAGE: Japanese

G1 For diagram(s), see printed CA Issue.

AB Thianaphthene (72.3 g.) added to BuLi from 8.2 g. Li, 79.8 g. BuBr, and 250 ml. Et2O at -20° and treated with 94.4 g. Br in 200 ml. Et2O at -70° gave 87 g. 2-bromothianaphthene (I). I (160.5 g.), 30.6 g. CuO, and 0.8 g. KI added to 49 g. Na in 660 ml. MeOH and heated 210 hrs. gave 75.7 g. 2-methoxythianaphthene (II), m. 41-2°, b17.5 140.5-1.5°. Similarly 3-methoxythianaphthene (III), b3 107-8.5°, d204 1.2001, n20D 1.6219, was obtained in 95.6% yield. II (16.4 g.) in 80 ml. CCl4 treated with 17.3 g. N-bromosuccinimide at 0° and then at room temperature gave 18.4 g. unstable 3-bromo-2-methoxythianaphthene (IV), b2 119-20°, m. 23.5°. Similarly 2-bromo-3-methoxythianaphthene (V), b3 123-5°, d204 1.5485, which was also unstable, was obtained. II (16.4 g.) in 26 ml. ligroin and 12.3 g. Ac2O treated with 13.2 ml. Et2O.BF3 at 55-65° gave 17.7 g. 3-acetyl-2-methoxythianaphthene (VI), m. 112-13°; oxime m. 134-5°. Similarly III gave 2-acetyl-3-methoxythianaphthene (VII), m. 66-7° (oxime m. 155-6°) in 49.7% yield. IV (4.9 g.) in 20 ml. PhNO2 treated with 1.7 g. AcCl and 2.9 g. AlCl3 at 0° gave 0.48 g. VI. Treating V in PhNO2 with AcCl and AlCl3 gave 55.5% thioindigo (VIII). Treating V with AlCl3 at 0° or Et2O.BF3 at the b.p. also gave VIII. Mechanism of formation of VIII is discussed. VI (2.06 g.) in 15 ml. AcOH treated with 4 ml. HNO3 (d. 1.40) at room temperature yielded 1.51 g. 3,4-bis(2-methoxy-3-thianaphthyl)carbonyl-1,2,5-oxadiazole 2-oxide, m. 204-5°. Similar reaction reaction of VII did not produce furazan derivative II (4.1 g.) in 5.5 g. HCONMe2 treated with 4.8 g. POC13 below 60° gave 3.1 g. 3-formyl-2-methoxythianaphthene (IX), m. 59-60°; semicarbazone m. 208-9°. Similarly 2-formyl-3-methoxythianaphthene (m. 84.5-5.5°; semicarbazone m. 222-3°) was obtained in 95.9% yield. IX (0.34 g.), 0.5 g. CH2(CO2H)2, 2 ml. pyridine, and 3 drops piperidine heated 6 hrs. at 100° and then 20 min. under reflux gave 0.36 g. 3-(2-methoxy-4-thianaphthyl)acrylic acid, m. 171-2°. Similarly 3-(3-methoxy-2-thianaphthyl)acrylic acid, m. 191-2°, was prepared. I (4.9 g.) in 8 ml. Et2O treated with PhLi from 0.45 g. Li, 5 g. PhBr, and 40 ml. Et2O and then with CO2 yielded 2 g. 2-methoxythianaphthene-3-carboxylic acid (X), m. 199-200°; Me ester m. 65.5-6.5°. Using BuLi instead of PhLi gave 64% X. Similarly 3-methoxythianaphthene-2-carboxylic acid, m. 176-7° (Me ester m. 64.5-5.5°) was obtained in 93.8% yield. II (1.6 g.) treated with BuLi from 1.5 g. BuBr and 0.2 g. Li and then with 3.2 g. CuCl2 at -30° gave 0.4 g. 2,2'-dimethoxy-3,3'-bithianaphthyl, m. 139-40°. Similarly 3,3'-dimethoxy-2,2'-bithianaphthyl, m. 175-6.5°, was obtained. III (0.5 g.) treated with 1.8 g. (AcO)2Hg in 12.5 ml. 50% AcOH yielded 1.2 g. 2-acetoxymercuri-3-methoxythianaphthene, m. 196.5-98°.

L3 ANSWER 12 OF 14 CAPLUS COPYRIGHT 2007 ACS ON STN
ACCESSION NUMBER: 1967:443677 CAPLUS
DOCUMENT NUMBER: 67:43677
TITLE: New benzothienophenes
PATENT ASSIGNEE(S): Aktiebolag Hassle, Apotekare Paul Nordstroms Fabriker
SOURCE: Neth. Appl., 16 pp.
CODEN: NAOXAN
DOCUMENT TYPE: Patent
LANGUAGE: Dutch
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
NL 6607608		19661202	NL 1966-7608	19660601
DE 1645913			DE	
FR 1481720			FR	
FR 5822			FR	
GB 1101946			GB	
SE 339235			SE	
US 3485835		19691223	US	19690410
US 3558616		19710126	US	19691110
US 3594478		19710720	US	19691124
US 3665074		19720523	US	19690520
			SE	19650601

PRIORITY APPLN. INFO:

OTHER SOURCE(S): HARPAT 67:43677

G1 For diagram(s), see printed CA Issue.

AB The preparation of the title compds. (I) and their acid addition salts is described. The title compds. are valuable pharmaceuticals, in particular because of their analgesic, antipyretic, antiinflammatory, antitussive, local anesthetic, antispasmodic, and antihistaminic activity. Thus, 15 g. 2-mercapto-5-methylbenzoic acid, 26 g. K2CO3, 22 g. o-bromo-p-ethoxyacetophenone, and 260 ml. Me2CO were stirred and refluxed overnight. H2O was added until a clear solution was obtained, the mixture was acidified, and the product filtered to give 18.9 g. o-[4-methyl-2-carboxyphenoxymethyl]-4-ethoxyacetophenone (II), m. 153° (alc.). Similarly prepared were the following o-[2-carboxyphenoxymethyl]-4-ethoxyacetophenones (III) (R0, R1, R2, and m.p. given): 4-OMe, H, H, 190°; 4-F, H, H, 166°; 4-Cl, H, H, 166°; 4-OMe, H, H, 180°; 4-OEt, H, H, 166°; 4-Me, 5-Me, H, 174°; 4-OEt, 6-Me, H, 190°; 4-OEt, 4-Me, 5-Me, 160°; 4-OEt, 4-Cl, H, 163°; 4-OEt, 6-Cl, H, 140°; and 4-OEt, 4-OMe, H, 154°. To an ice-cold solution of 5.6 g. diazomethane in 250 ml. Et2O was added 29.4 g. II, the mixture brought to room temperature over

2 hrs., the Et2O evaporated, and the residue recrystd. from MeOH to give 31.2 g.

9. o-[4-methyl-2-carboxyphenoxymethyl]-4-ethoxyacetophenone (IV). The following o-[2-carboxyphenoxymethyl]-4-ethoxyacetophenones (V) were prepared (R0, R1, R2, and m.p. given): 4-OMe, H, H, 58°; 4-F, H, H, 114°; 4-Cl, H, H, 130°; 4-OMe, H, H, 136°; 4-OEt, H, H, 108°; 4-Me, 5-Me, H, 105°; 4-OEt, 6-Me, H, 108°; 4-OEt, 4-Me, 5-Me, 107°; 4-OEt, 4-Cl, H, 102°; 4-OEt, 6-Cl, H, 66°; and 4-OEt, 4-OMe, H, 120°. Na (2.5 g.) was dissolved in 200 ml. absolute alc., 31 g. IV added, and the mixture stirred and refluxed 2 hrs., poured onto ice water, and acidified to give 25.5 g. of a product, m. 140°. Similarly prepared were the following 2-aryl-3-hydroxybenzothienophenes, VI (R0, R1, R2, and m.p. given): 4-OMe, H, H, 93°; 4-F, H, H, 115°; 4-Cl, H, H, 150°; 4-OMe,

L3 ANSWER 12 OF 14 CAPLUS COPYRIGHT 2007 ACS ON STN (Continued)
H, H, 112°; 4-OEt, H, H, 140°; H, 6-Me, H, 105°; 4-OEt, 5-Me, 6-Me, 177°; 4-OEt, 5-Cl, H, 154°; 4-OEt, 7-Cl, H, 134°; 4-OEt, 5-OMe, H, 150°. To a soln. of 30 g. 3-methoxybenzothienophene and 35 g. p-ethoxybenzoyl chloride in 200 ml. CS2 was added 30 g. anhyd. AlCl3, the mixt. refluxed 3 hrs. and distd. to remove the solvent, the residue acidified with 5N HCl, and the mixt. extd. with Et2O to give 25.2 g. product, m. 139° (MeCOEt). Similarly prepd. were the following VI (R0, R1, R2, and m.p. given): H, H, H, 119°; 4-F, H, H, 116°; 4-Cl, H, H, 170°. Salicylic acid (20 g.) was added to 200 ml. concd. H2SO4, 24 g. benzoylacetone added, the mixt. heated 1 hr. at 50°, poured into ice water, and worked up to give 19 g. 2-benzoyl-3-hydroxybenzothienophene (VII), m. 116°. A mixt. of 12 g. VII, 120 ml. Me2CO, 19.5 g. K2CO3, and 7.5 g. 2-dimethylaminoethyl chloride hydrochloride was refluxed 24 hrs., filtered, and worked up with Et2O to give 4.7 g. 2-benzoyl-3-N,N-dimethylaminoethoxybenzothienophene-HCl, m. 138°. Similarly prepd. were: 2-(p-ethoxybenzoyl)-3-pyrrolidinoethoxy-5-methylbenzothienophene-HCl, m. 169°; 2-(p-tert-butylbenzoyl)-3-pyrrolidinoethoxybenzothienophene-HCl, m. 162°. A mixt. of 8.4 g. p-toluenesulfonyl chloride, 200 ml. Me2CO and 5.1 g. pyrrolidinoethanol was refluxed for 10 min., cooled, 12.5 g. 2-(p-ethoxybenzoyl)-3-hydroxy-5-methylbenzothienophene (VIII) and 16.6 g. K2CO3 added, and the mixt. refluxed overnight, worked up, and acidified to give 2-(p-ethoxybenzoyl)-3-pyrrolidinoethoxy-5-methylbenzothienophene-HCl, m. 169°. Refluxing of a mixt. of 9 g. VIII, 200 ml. Me2CO, and 10.8 g. 2-pyrrolidinoethyl chloride overnight, addn. of 10 g. K2CO3, and work-up gave a product, m. 169° (Me2CO). Similarly, refluxing overnight of 12 g. 2-benzoyl-3-hydroxybenzothienophene, 120 ml. Et3B, and 705 g. dimethylaminoethyl chloride hydrochloride and addn. of 20 g. K2CO3 gave a product, m. 138° (EtOAc). Also prepd. were: 2-(p-ethoxybenzoyl)-3-pyrrolidinoethoxybenzothienophene-HCl, m. 137-40°; 2-(p-ethoxybenzoyl)-3-pyrrolidinoethoxy-5-methylbenzothienophene-HCl, m. 169°; 2-benzoyl-3-N,N-diethylaminoethoxybenzothienophene-HCl, m. 107° and 2-(p-ethoxybenzoyl)-3-pyrrolidinoethoxy-5-methylbenzothienophene-HCl, m. 169°. The following I (A = CH2CH2, R = 2-substituted benzyl) were prepd. similarly (Z, R1, R2, NR3R4, and m.p. given): H, H, H, 152°; 135°; H, H, H, 152°; p-iso-Pr, H, H, 1-pyrrolidinyl, 162°; p-F, H, H, 152°; p-F, H, H, 1-pyrrolidinyl, 177°; p-Cl, H, H, 152°; p-Cl, H, H, 1-pyrrolidinyl, 196°; p-Cl, H, H, 43-piperidino, 215°; p-Cl, H, H, piperidino, 144°; p-OMe, H, H, 152°; 130°; p-OMe, H, H, 1-pyrrolidinyl, 177°; p-OMe, H, H, 43-piperidino, 190°; p-OMe, H, H, piperidino, 128°; p-OEt, H, H, 152°; 150°; p-OEt, H, H, 1-pyrrolidinyl, 140°; p-OEt, H, H, piperidino, 180°; p-OEt, H, H, morpholino, 165°; p-OEt, 5-Me, H, 152°; 187°; p-OEt, 5-Me, H, 1-pyrrolidinyl, 169°; p-OEt, 5-Me, H, piperidino, 157°; H, H, 6-Me, 1-pyrrolidinyl, 166°; p-OEt, 5-Me, 6-Me, 1-pyrrolidinyl, 104°; p-OEt, 5-Cl, H, 1-pyrrolidinyl, 149°; p-OEt, 7-Cl, H, piperidino, 180°; p-OEt, 5-OMe, H, 1-pyrrolidinyl, 93°; p-OEt, 5-OMe, H, morpholino, 121°. The prepn. of pharmaceutical compns. contg. the compds. prepd. was described.

L3 ANSWER 13 OF 14 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1949:10919 CAPLUS
DOCUMENT NUMBER: 43:10919
ORIGINAL REFERENCE NO.: 43:2200d-1, 2201a-e
TITLE: Derivatives of 3-hydroxythianaphthene
AUTHOR(S): Rodionov, V. M.; Bogoslovskii, B. M.; Kazakova, Z. S.
SOURCE: Izvestiya Akademii Nauk SSSR, Seriya Khimicheskaya
(1948) 536-47
CODEN: IASKA6; ISSN: 0002-3353

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

G1 For diagram(s), see printed CA issue.

AB o-HSC6H4CO2H (I) (3 g.), 2 g. ClCH2Ac, and 6.6 g. crystalline NaOAc in 100 ml. EtOH, let stand 10 hrs., then diluted with 200 ml. H2O, acidified by HCl, and concentrated to 150 ml. give 80.7% 5-acetylthiosalicylic acid, m. 153-4° (from EtOH); this is obtained also in 78% yield by heating to 100° 2 hrs. 7.6 g. (o-HO2CC6H4)2S (II), 6 g. ClCH2Ac, 10 ml. 40% NaOH, 20 ml. water, and 10 ml. EtOH. I (6 g.), 3.7 g. ClCH2Ac, and 6.5 g. dry NaOH in 100 ml. absolute EtOH heated 10 hrs. on a steam bath, concentrated to 0.5 volume, poured into ice water, and acidified by HCl, give 86%

2-acetyl-3-hydroxythianaphthene, m. 81° (from 40% EtOH), soluble in dilute NaOH. This (1 g.) heated with Ac2O gives 2,3-diacetyl-3-hydroxythianaphthene, yellow, m. 126° (from EtOH). I (3.2 g.), 3.2 g. BrCH2Cl, and 5.4 g. crystalline NaOAc let stand 6 hrs. in 100 ml. EtOH, followed by dilution with water, give 89% 2-BrCH2SC6H4CO2H, m. 182° (from 50% EtOH); similar reaction using 3.3 g. dry NaOAc at reflux for 20 hrs. gives 75% 2-benzoyl-3-hydroxythianaphthene, yellow, m. 118° (from EtOH), soluble in hot 5% NaOH; the 3-Ac derivative, made with Ac2O, m. 105° (from EtOH). II (7.6 g.) or 7.7 g. I in 20 ml. water and 10 ml. 40% NaOH, treated with 10 g. BrCH2CH(OMe)2 in 10 ml. EtOH, followed by 2 hrs. heating, cooling, and acidification by HCl on dilution, give 63% o-HO2CC6H4SCH2CH(OMe)2, m. 114-15° (from C6H6), which with a trace of warm dilute acids reverts to the aldehyde, o-HO2CC6H4SCH2CHO (III), m. 156°, best obtained (90%) by solution of 1.5 g. I, 2 g. BrCH2CH(OMe)2, and 2.6 g. crystalline NaOAc in 50 ml. EtOH and treatment with 150 ml. cold H2O and 3-4 ml. concentrated HCl, followed by 1

hr. on a steam bath and concentration; on crystallization from water it gives a dihydrate, m.

159°, while on treatment with NH3-AgO it gives o-HO2CC6H4SCH2CO2H, m. 213°. III gives the oxime, m. 152° (from 50% EtOH). III (0.8 g.) in 10 ml. EtOH and 0.15 g. N2H4.H2O, let stand 1.0 hr. and heated 0.5 hr., followed by cooling and dilution, give 54% azine derivative (o-HO2CC6H4SCH2CH=N)2, m. 147° (from 50% EtOH). III gives a semicarbazone, m. 165° (from 50% NaOH). III oxime (4.5 g.) heated with 30 ml. Ac2O 1 hr. to 100°, followed by heating with 0.75 g. P2O5 and treatment with water, gives the nitrile, o-HO2CC6H4SCH2CN, m. 195-8° (from AcOH, then PhMe); use of SOCl2 in this preparation gives a cyanine dye, which can be prepared in 90%

yield by heating 3-hydroxythianaphthene to 100° with 100% HCO2H; the red product, CO.C6H4.S.CHCH2C.S.C6H4.CO, decompose 270° (from EtOH). III (1 g.), 0.9 g. hippuric acid, and 1.6 g. dry NaOAc with 20 ml. Ac2O heated 0.5 hr. give 88.7% of the oxazolone, o-HO2CC6H4SCH2CH:C.NiCPh.O.CO, m. 230° (from AcOH), on cooling and dilution with EtOH. III (2 g.) boiled 10 min. with 15 ml. Ac2O, then poured on ice, gives 62% 2-formyl-3-hydroxythianaphthene, yellowish, m. 107° (from 30% EtOH), which gives the Ag mirror test only in the absence of NaOH; the latter (1.8 g.) in 50% AcOH treated with 1 g. N2H4.H2O gives 66% azine derivative, [S.C6H4.C(OH):CCH=N]2, yellow, m.

L3 ANSWER 14 OF 14 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1941:30357 CAPLUS
DOCUMENT NUMBER: 35:30357
ORIGINAL REFERENCE NO.: 35:4769g-1, 4770a
TITLE: Dismutation of some disulfides. IV
AUTHOR(S): Fowkes, F. S.; McClelland, E. W.
SOURCE: Journal of the Chemical Society (1941) 187-90
CODEN: JCSOA9; ISSN: 0368-1769

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB cf. C. A. 28, 5439.9. It is shown that Cl in the p-position to S decreases the tendency of 2,2'-bithiobenzoic acid (I) to undergo dismutation. In consequence the 5,5'-di-Cl derivative (II) of I reacts less readily than I with Ac2CH2 in H2SO4 but yields similar products. II (1 g.), 1.25 g. AcOK and 12 cc. Ac2O, heated 4 hrs. at 130° (little reaction at 125° in 2 hrs.) and the product distilled with steam at 100°, give 0.05 g. 5-chloro-3-hydroxy-2-acetyl-1-thianaphthene (III), yellow, m. 166°, and 0.2 g. of 5-chloro-3-acetoxy-1-thianaphthene (IV), m. 67°. Reaction of 0.56 g. Ac2CH2 (added during 1 hr.) with 1 g. II in 8 cc. concentrated H2SO4 for 40 min. at 50-5° gives 0.75 g. III; it gives an olive-green color with FeCl3 in EtOH. Refluxing III with Ac2O in PhMe containing a trace of CSH5N for 6 hrs. gives the 3-Ac derivative, m.

132°; 3-acetoxy-2-acetyl-1-thianaphthene, m. 127°. Refluxing 1 g. III and 1.45 g. PhNHNH2 in C6H6 for 3 hrs. gives the hydrazone, yellow, m. 162°; boiling in EtOH containing 1 drop of concentrated

H2SO4 for 30 min. gives 8-chloro-1-phenyl-3-methyl-4,5-thianaphthenopyrazole, m. 135°. III with H2O2-AcOH (3 days at room temperature) gives the 1,1-dioxide, m. 265°. 5-Chloro-3-hydroxy-1-thianaphthene and PhNHNH2 in AcOH, heated at 100° for 35 min., give 10-chlorothianaphthindole, m. 222°; IV gives the same product; isatin in H2SO4 gives a blue color. H2O2 in AcOH transforms IV (4.5 days, with frequent shaking) into the 1,1-dioxide, m. 164°; if the reaction is heated at 100° for 1 hr. there results 5-chloro-3-hydroxy-1-thianaphthene 1,1-dioxide, m. 194°; the hydrazone, yellow, m. 290-2°. could be indolized. Refluxing 30 g. I in 1 l. xylene with 20 g. P2S5 for 6 hrs. gives 75% of 2,3-dithiosulfindene; this reaction suggests that I undergoes dismutation in neutral as well as in acid media.

L3 ANSWER 13 OF 14 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

198° (from C6H6); use of EtOH solvent always gives the cyanine dye described above. The formyl deriv. yields a semicarbazone, m. 185° (from 20% EtOH).

L3 ANSWER 10 OF 14 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1970:121469 CAPLUS
DOCUMENT NUMBER: 72:121469
TITLE: Rearrangement of benzothiazine sulfoxides
AUTHOR(S): Morin, Robert B.; Spry, Douglas O.
CORPORATE SOURCE: Lilly Res. Lab., Eli Lilly and Co., Indianapolis, IN, USA
SOURCE: Journal of the Chemical Society [Section] D: Chemical Communications (1970), (6), 335-6
CODEN: CCJDAO; ISSN: 0577-6171

DOCUMENT TYPE:

LANGUAGE: English
GI For diagram(s), see printed CA Issue.

AB Reaction of substituted benzothiazine sulfoxides with Ac₂O under reflux leads by an elimination reaction to a sulfenic acid derivative that

undergoes

subsequent addition to the double bond formed if the N is tertiary but is trapped as a cyclic sulfenamide by a secondary N. Oxidizing I (R = H) with m-ClC₆H₄CO₂H (II) in CHCl₃ at -8° gave the sulfoxide, m. 128-9°, which was refluxed with Ac₂O containing 1% NaOAc to give a 3:2 mixture of III [R = CMe:CH₂] (III), presumably via IV, and V [R = H] (IX). Refluxing the sulfoxide of I (R = Me), m. 80-2°, with Ac₂O-NaOAc gave 50% VI [R = C(OAc):CH₂] (VII), variable yields of the interconvertible VI (R = H) and VIII (neither of which gave VII under the reaction conditions), and approx. 10% V (R = Ac), all via IV (R = Me) (IX). Acetylation of the enamide IX followed by addition of the sulfenic group to the substituted double bond and enol acetylation presumably gave VII. The sole oxidation product from X by oxidation with II at room

temperature or

using O₃ at -70° was III (R = Me), apparently via the sulfoxide followed by elimination; the generated sulfenic acid reacts with the neighboring amide group.

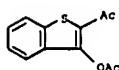
IT 27468-08-2P

RL: SPN (Synthetic preparation); PREP (Preparation)

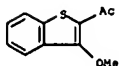
(preparation of)

RN 27468-08-2 CAPLUS

CN Ketone, 3-hydroxybenzo[b]thien-2-yl methyl, acetate (8CI) (CA INDEX NAME)



L3 ANSWER 11 OF 14 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CN Ketone, 3-methoxybenzo[b]thien-2-yl methyl (8CI) (CA INDEX NAME)



L3 ANSWER 11 OF 14 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1968:467165 CAPLUS
DOCUMENT NUMBER: 69:67165
TITLE: Syntheses of 2-methoxy- and 3-methoxythianaphthenes
AUTHOR(S): Matsuki, Yasuo; Adachi, Yoshio
CORPORATE SOURCE: Tohoku Univ., Sendai, Japan
SOURCE: Nippon Kagaku Zasshi (1968), 89(2), 192-6
CODEN: NPKZAZ; ISSN: 0369-5387

DOCUMENT TYPE:

LANGUAGE: Japanese
GI For diagram(s), see printed CA Issue.

AB Thianaphthene (72.3 g.) added to BuLi from 8.2 g. Li, 79.8 g. BuBr, and 250 ml. Et₂O at -20° and treated with 94.4 g. Br in 200 ml. Et₂O at -70° gave 87 g. 2-bromothianaphthene (I). I (160.5 g.), 30.6 g. CuO, and 0.8 g. KI added to 49 g. Na in 660 ml. MeOH and heated 210 hrs. gave 75.7 g. 2-methoxythianaphthene (II), m. 41-2°, b_{17.5} 140.5-1.5°. Similarly 3-methoxythianaphthene (III), b₃ 107-8.5°, d₂₀ 1.2001, n_D 1.6219, was obtained in 95.6% yield. II (16.4 g.) in 80 ml. CCl₄ treated with 17.3 g. N-bromosuccinimide at 0° and then at room temperature gave 18.4 g. unstable 3-bromo-2-methoxythianaphthene (IV), b₂ 119-20°, m. 23.5°. Similarly 2-bromo-3-methoxythianaphthene (V), b₃ 123-5°, d₂₀ 1.5485, which was also unstable, was obtained. II (16.4 g.) in 26 ml. ligroin and 12.3 g. Ac₂O treated with 13.2 ml. Et₂O.BF₃ at 55-65° gave 17.7 g. 3-acetyl-2-methoxythianaphthene (VI), m. 112-13°; oxime m. 134-5°. Similarly III gave 2-acetyl-3-methoxythianaphthene (VII), m. 66-7° (oxime m. 155-6°) in 49.7% yield. IV (4.9 g.) in 20 ml. PhNO₂ treated with 1.7 g. AcCl and 2.9 g. AlCl₃ at 0° gave 0.48 g. VI. Treating V in PhNO₂ with AcCl and AlCl₃ gave 55.5% thioindigo (VIII). Treating V with AlCl₃ at 0° or Et₂O.BF₃ at the b.p. also gave VIII. Mechanism of formation of VIII is discussed. VI (2.06 g.) in 15 ml. AcOH treated with 4 ml. HNO₃ (d. 1.40) at room temperature yielded 1.51 g.

3,4-bis(2-methoxy-3-thianaphthylcarbonyl)-1,2,5-oxadiazole 2-oxide, m. 204-5°. Similar reaction reaction of VII did not produce furazan derivative II (4.1 g.) in 5.5 g. HCONMe₂

treated with 4.8 g. POC₃ below 60° gave 3.1 g. 3-formyl-2-methoxythianaphthene (IX), m. 59-60°; semicarbazone m. 208-9°. Similarly 2-formyl-3-methoxythianaphthene (m. 84.5-5.5°; semicarbazone m. 222-3°) was obtained in 95.9% yield. IX (0.34 g.), 0.5 g. CH₂(CO₂H)₂, 2 ml. pyridine, and 3 drops piperidine heated 6 hrs. at 100° and then 20 min. under reflux gave 0.36 g. 3-(2-methoxy-4-thianaphthyl)acrylic acid, m. 171-2°. Similarly 3-(3-methoxy-2-thianaphthyl)acrylic acid, m. 191-2°, was prepared. II (4.9 g.) in 8 ml. Et₂O treated with PhLi from 0.45 g. Li, 5 g. PhBr, and 40 ml. Et₂O and then with CO₂ yielded 2 g. 2-methoxythianaphthene-3-carboxylic acid (X), m. 199-200°; Me ester m. 65.5-6.5°. Using BuLi instead of PhLi gave 64% X. Similarly 3-methoxythianaphthene-2-carboxylic acid, m. 176-7° (Me ester m. 64.5-5.5°) was obtained in 93.8% yield. II (1.6 g.) treated with BuLi from 1.5 g. BuBr and 0.2 g. Li and then with 3.2 g. CuCl₂ at -30° gave 0.4 g. 2,2'-dimethoxy-3,3'-bithianaphthyl, m. 139-40°. Similarly 3,3'-dimethoxy-2,2'-bithianaphthyl, m. 175.5-6.5°, was obtained. III (0.5 g.) treated with 1.8 g. (AcO)₂Zn in 12.5 ml. 50% AcOH yielded 1.2 g. 2-acetoxymercuri-3-methoxythianaphthene, m. 196.5-98°.

IT 19354-38-2P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

RN 19354-38-2 CAPLUS

L3 ANSWER 12 OF 14 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1967:443677 CAPLUS
DOCUMENT NUMBER: 67:43677
TITLE: New benzothienophenes
PATENT ASSIGNEE(S): Aktiebolag Hassle, Apotekare Paul Nordstroms Fabrikker
SOURCE: Meth. Appl., 16 pp.
CODEN: NAXXAN
DOCUMENT TYPE: Patent
LANGUAGE: Dutch
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
NL 6607608		19661202	NL 1966-7608	19660601
DE 1645913			DE	
FR 1481720			FR	
FR 5822			FR	
GB 1101946			GB	
SE 339235			SE	
US 3485835		19691223	US	19690410
US 3558616		19710126	US	19691110
US 3594478		19710720	US	19691124
US 3665074		19720523	US	19690520
			SE	19650601

PRIORITY APPLN. INFO.:

OTHER SOURCE(S): MARPAT 67:43677

GI For diagram(s), see printed CA Issue.

AB The preparation of the title compds. (I) and their acid addition salts is described. The title compds. are valuable pharmaceuticals, in particular because of their analgesic, antipyretic, antiinflammatory, antitussive, local anesthetic, antispasmodic, and antihistaminic activity. Thus, 15 g. 2-mercapto-5-methylbenzoic acid, 26 g. K₂CO₃, 22 g. o-bromo-p-ethoxyacetophenone, and 260 ml. Me₂CO were stirred and refluxed overnight, H₂O was added until a clear solution was obtained, the mixture was acidified,

and the product filtered to give 18.9 g. o-[4-methyl-2-carboxythiophenoxy]-4-ethoxyacetophenone (II), m. 153° (alc.). Similarly prepared were the following o-[2-carboxythiophenoxy]acetophenones (III) (R₁, R₂, and m.p. given): 4-CMe₃, H, H, 190°; 4-F, H, H, 166°; 4-Cl, H, H, 166°; 4-OMe, H, H, 180°; 4-OEt, H, H, 166°; 4-Me, 5-Me, H, 174°; 4-OEt, 6-Me, H, 190°; 4-OEt, 4-Me, 5-Me, 160°; 4-OEt, 4-Cl, H, 163°; 4-OEt, 6-Cl, H, 140°; and 4-OEt, 4-OMe, H, 154°. To an ice-cold solution of 5.6 g. diazomethane in 250 ml. Et₂O was added 29.4 g. II, the mixture brought to room temperature over

2

hrs., the Et₂O evaporated, and the residue recrystd. from MeOH to give 31.2 g. o-[4-methyl-2-carboxythiophenoxy]-4-ethoxyacetophenone (IV). The following o-[2-carboxythiophenoxy]acetophenones (V) were prepared (R₁, R₂, and m.p. given): 4-CMe₃, H, H, 59°; 4-F, H, H, 114°; 4-Cl, H, H, 130°; 4-OMe, H, H, 136°; 4-OEt, H, H, 108°; 4-Me, 5-Me, H, 105°; 4-OEt, 6-Me, H, 108°; 4-OEt, 4-Cl, H, 107°; 4-OEt, 4-Cl, H, 102°; 4-OEt, 6-Cl, H, 66°; and 4-OEt, 4-OMe, H, 120°. Na (2.5 g.) was dissolved in 200 ml. absolute alc., 31 g. IV added, and the mixture stirred

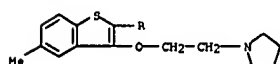
and

refluxed 2 hrs., poured onto ice water, and acidified to give 25.5 g. of a product, m. 140°. Similarly prepared were the following 2-aryl-3-hydroxybenzothienophenes, VI (R₁, R₂, and m.p. given): 4-CMe₃, H, H, 93°; 4-F, H, H, 115°; 4-Cl, H, H, 150°; 4-OMe,

L3 ANSWER 12 OF 14 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
 H, H, 112'; 4-OEt, H, H, 140'; H, 6-Me, H, 105';
 4-OEt, 5-Me, 6-Me, 177'; 4-OEt, 5-Cl, H, 154'; 4-OEt, 7Cl,
 H, 134'; 4-OEt, 5-OMe, H, 150'. To a soln. of 30 g.
 3-methoxybenzothiophene and 35 g. p-ethoxybenzoyl chloride in 200 ml. CS₂
 was added 30 g. anhyd. AlCl₃, the mixt. refluxed 3 hrs. and the mixt. extd.
 with Et₂O to give 25.2 g. product, m. 139° (MeCOEt). Similarly
 prepd. were the following VI (R₁, R₂, and m.p. given): H, H, H,
 119'; 4-F, H, H, 116'; 4-Cl, H, H, 170'. Salicylic
 acid (20 g.) was added to 200 ml. concd. H₂SO₄, 24 g. benzoylacetone
 added, the mixt. heated 1 hr. at 50°, poured into ice water, and
 worked up to give 19 g. 2-benzoyl-3-hydroxybenzothiophene (VII), m.
 116°. A mixt. of 12 g. VII, 120 ml. Me₂CO, 19.5 g. K₂CO₃, and 7.5
 g. 2-dimethylaminoethyl chloride hydrochloride was refluxed 24 hrs.,
 filtered, and worked up with Et₂O to give 4.7 g. 2-benzoyl-3-N,N-
 dimethylaminoethoxybenzothiophene-HCl, m. 138°. Similarly prepd.
 were: 2-(p-ethoxybenzoyl) - 3 - pyrrolidinoethoxy - 5 -
 methylbenzothiophene - HCl, m. 169'; 2-(p-tert-butylbenzoyl) - 3 -
 pyrrolidinoethoxybenzothiophene-HCl, m. 162'. A mixt. of 8.4 g.
 p-toluenesulfonyl chloride, 200 ml. Me₂CO and 5.1 g. pyrrolidinoethanol
 was refluxed for 10 min., cooled, 12.5 g. 2-(p-ethoxybenzoyl)-3-hydroxy-5-
 methylbenzothiophene (VIII) and 16.6 g. K₂CO₃ added, and the mixt.
 refluxed overnight, worked up, and acidified to give 2-(p-ethoxybenzoyl) -
 3 - pyrrolidinoethoxy - 5 - methylbenzothiophene-HCl, m. 169'.
 Refluxing of a mixt. of 9 g. VIII, 200 ml., Me₂CO, and 10.8 g.
 2-pyrrolidinoethyl chloride overnight, addn. of 10 g. K₂CO₃, and work-up
 gave a product, m. 169° (Me₂CO). Similarly, refluxing overnight of
 12 g. 2-benzoyl-3-hydroxybenzothiophene, 120 ml. Et₃N, and 705 g.
 dimethylaminoethyl chloride hydrochloride and addn. of 20 g. K₂CO₃ gave a
 product, m. 138° (EtOAc). Also prepd. were: 2-(p-ethoxybenzoyl)-3-
 pyrrolidinoethoxybenzothiophene-HCl, m. 137-40';
 2-(p-ethoxybenzoyl) - 3 - pyrrolidinoethoxy - 5 - methylbenzothiophene -
 HCl, m. 169'; 2-benzoyl-3-N,N-dimethylaminoethoxybenzothiophene-HCl,
 m. 107° and 2-(p-ethoxybenzoyl)-3-pyrrolidinoethoxy-5-
 methylbenzothiophene-HCl, m. 169'. The following I (A = CH₂CH₂, R
 = 2-substituted benzyl) were prepd. similarly (Z, R₁, R₂, NR₃R₄, and m.p.
 given): H, H, H, Me₂, 135'; H, H, H, NEt₂, 112'; p-iso-Pr,
 H, H, 1-pyrrolidinyl, 162'; p-F, H, H, NEt₂, 159'; p-F, H,
 H, 1-pyrrolidinyl, 177'; p-Cl, H, H, NEt₂, 187'; p-Cl, H, H,
 1-pyrrolidinyl, 196'; p-Cl, H, H, Δ³-piperidino, 215';
 p-Cl, H, H, piperidino, 144'; p-OMe, H, H, NEt₂, 130';
 p-OMe, H, H, 1-pyrrolidinyl, 177'; p-OMe, H, H,
 Δ³-piperidino, 190'; p-OMe, H, H, piperidino, 128';
 p-OEt, H, H, NEt₂, 150'; p-OEt, H, H, 1-pyrrolidinyl, 140';
 p-OEt, H, H, piperidino, 180'; p-OEt, H, H, morpholino,
 165'; p-OEt, 5-Me, H, NEt₂, 187'; p-OEt, 5-Me, H,
 1-pyrrolidinyl 169'; p-OEt, 5-Me, H, piperidino, 157'; H, H,
 6-Me, 1-pyrrolidinyl, 166'; p-OEt, 5-Me, 6-Me, 1-pyrrolidinyl,
 104'; p-OEt, 5-Cl, H, 1-pyrrolidinyl, 149'; p-OEt, 7-Cl, H,
 piperidino, 180'; p-OEt, 5-OMe, H, 1-pyrrolidinyl, 93';
 p-OEt, 5-OMe, H, morpholino, 121'. The prepn. of pharmaceutical
 compns. containing the compds. prepd. was described.

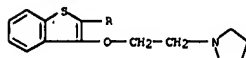
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 15776-49-5P 15776-50-8P 15776-51-9P
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L3 ANSWER 12 OF 14 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



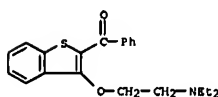
● HCl

RN 15776-33-7 CAPLUS
 CN Ketone, p-ethoxyphenyl 3-[2-(1-pyrrolidinyl)ethoxy]benzo[b]thien-2-yl,
 hydrochloride (8C1) (CA INDEX NAME)



● HCl

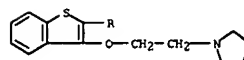
RN 15776-34-8 CAPLUS
 CN Ketone, 3-[2-(diethylamino)ethoxy]benzo[b]thien-2-yl phenyl, hydrochloride
 (8C1) (CA INDEX NAME)



● HCl

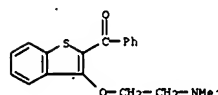
RN 15776-35-9 CAPLUS
 CN Ketone, p-tert-butylphenyl 3-[2-(1-pyrrolidinyl)ethoxy]benzo[b]thien-2-yl

L3 ANSWER 12 OF 14 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
 15897-65-1P 15897-66-2P 15897-67-3P
 15897-68-4P 15897-69-5P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)
 RN 15776-29-1 CAPLUS
 CN Ketone, p-tert-butylphenyl 3-[2-(1-pyrrolidinyl)ethoxy]benzo[b]thien-2-yl,
 hydrochloride (8C1) (CA INDEX NAME)



● HCl

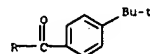
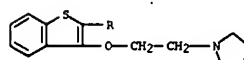
RN 15776-30-4 CAPLUS
 CN Ketone, 3-[2-(dimethylamino)ethoxy]benzo[b]thien-2-yl phenyl,
 hydrochloride (8C1) (CA INDEX NAME)



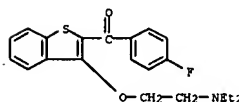
● HCl

RN 15776-31-5 CAPLUS
 CN Ketone, p-ethoxyphenyl 5-methyl-3-[2-(1-pyrrolidinyl)ethoxy]benzo[b]thien-
 2-yl, hydrochloride (8C1) (CA INDEX NAME)

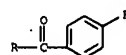
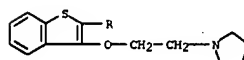
L3 ANSWER 12 OF 14 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



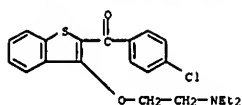
RN 15776-36-0 CAPLUS
 CN Ketone, p-ethoxyphenyl 3-[2-(1-pyrrolidinyl)ethoxy]benzo[b]thien-2-yl p-fluorophenyl (8C1)
 (CA INDEX NAME)



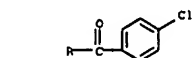
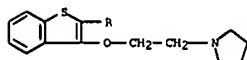
RN 15776-37-1 CAPLUS
 CN Ketone, p-fluorophenyl 3-[2-(1-pyrrolidinyl)ethoxy]benzo[b]thien-2-yl
 (8C1) (CA INDEX NAME)



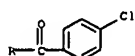
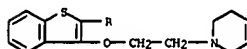
RN 15776-38-2 CAPLUS
 CN Ketone, p-chlorophenyl 3-[2-(diethylamino)ethoxy]benzo[b]thien-2-yl (8C1)
 (CA INDEX NAME)



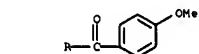
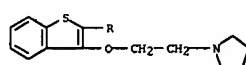
RN 15776-39-3 CAPLUS
CN Ketone, p-chlorophenyl 3-[2-(1-pyrrolidinyl)ethoxy]benzo[b]thien-2-yl (8CI) (CA INDEX NAME)



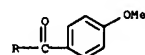
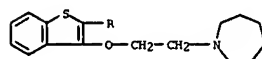
RN 15776-40-6 CAPLUS
CN Ketone, p-chlorophenyl 3-[2-(3,6-dihydro-1(2H)-pyridyl)ethoxy]benzo[b]thien-2-yl (8CI) (CA INDEX NAME)



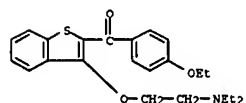
RN 15776-41-7 CAPLUS
CN Ketone, p-methoxyphenyl 3-[2-(1-pyrrolidinyl)ethoxy]benzo[b]thien-2-yl (8CI) (CA INDEX NAME)



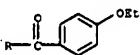
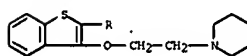
RN 15776-42-8 CAPLUS
CN Ketone, 3-[2-(hexahydro-1H-azepin-1-yl)ethoxy]benzo[b]thien-2-yl p-methoxyphenyl (8CI) (CA INDEX NAME)



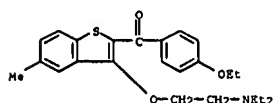
RN 15776-43-9 CAPLUS
CN Ketone, 3-[2-(diethylamino)ethoxy]benzo[b]thien-2-yl p-ethoxyphenyl (8CI) (CA INDEX NAME)



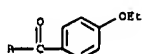
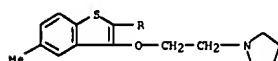
RN 15776-44-0 CAPLUS
CN Ketone, p-ethoxyphenyl 3-(2-piperidinoethoxy)benzo[b]thien-2-yl (8CI) (CA INDEX NAME)



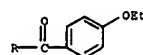
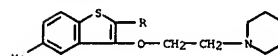
RN 15776-45-1 CAPLUS
CN Ketone, 3-[2-(diethylamino)ethoxy]-5-methylbenzo[b]thien-2-yl p-ethoxyphenyl (8CI) (CA INDEX NAME)



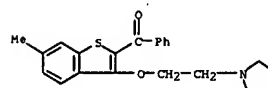
RN 15776-46-2 CAPLUS
CN Ketone, p-ethoxyphenyl 5-methyl-3-[2-(1-pyrrolidinyl)ethoxy]benzo[b]thien-2-yl (8CI) (CA INDEX NAME)



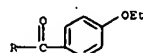
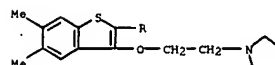
RN 15776-47-3 CAPLUS
CN Ketone, p-ethoxyphenyl 5-methyl-3-(2-piperidinoethoxy)benzo[b]thien-2-yl (8CI) (CA INDEX NAME)



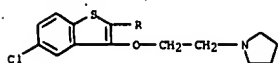
RN 15776-49-5 CAPLUS
CN Ketone, 6-methyl-3-[2-(1-pyrrolidinyl)ethoxy]benzo[b]thien-2-yl phenyl (8CI) (CA INDEX NAME)



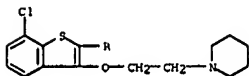
RN 15776-50-8 CAPLUS
CN Ketone, 5,6-dimethyl-3-[2-(1-pyrrolidinyl)ethoxy]benzo[b]thien-2-yl p-ethoxyphenyl (8CI) (CA INDEX NAME)



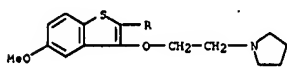
RN 15776-51-9 CAPLUS
CN Ketone, 5-chloro-3-[2-(1-pyrrolidinyl)ethoxy]benzo[b]thien-2-yl p-ethoxyphenyl (8CI) (CA INDEX NAME)



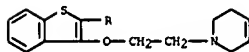
RN 15776-52-0 CAPLUS
CN Ketone, 7-chloro-3-(2-piperidinoethoxy)benzo[b]thien-2-yl p-ethoxyphenyl (8CI) (CA INDEX NAME)



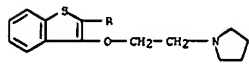
RN 15776-53-1 CAPLUS
CN Ketone, p-ethoxyphenyl 5-methoxy-3-[2-(1-pyrrolidinyl)ethoxy]benzo[b]thien-2-yl (8CI) (CA INDEX NAME)



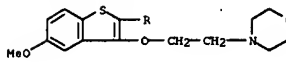
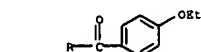
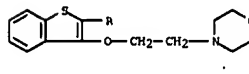
RN 15776-54-2 CAPLUS
CN Ketone, p-ethoxyphenyl 5-methoxy-3-(2-morpholinoethoxy)benzo[b]thien-2-yl (8CI) (CA INDEX NAME)



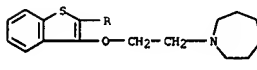
RN 15897-68-4 CAPLUS
CN Ketone, p-ethoxyphenyl 3-[2-(1-pyrrolidinyl)ethoxy]benzo[b]thien-2-yl (8CI) (CA INDEX NAME)



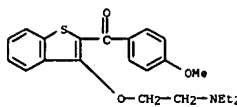
RN 15897-69-5 CAPLUS
CN Ketone, p-ethoxyphenyl 3-(2-morpholinoethoxy)benzo[b]thien-2-yl (8CI) (CA INDEX NAME)



RN 15897-65-1 CAPLUS
CN Ketone, p-chlorophenyl 3-[2-(hexahydro-1H-azepin-1-yl)ethoxy]benzo[b]thien-2-yl (8CI) (CA INDEX NAME)



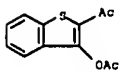
RN 15897-66-2 CAPLUS
CN Ketone, 3-[2-(diethylamino)ethoxy]benzo[b]thien-2-yl p-methoxyphenyl (8CI) (CA INDEX NAME)



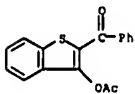
RN 15897-67-3 CAPLUS
CN Ketone, 3-[2-(3,6-dihydro-1(2H)-pyridyl)ethoxy]benzo[b]thien-2-yl p-methoxyphenyl (8CI) (CA INDEX NAME)

ACCESSION NUMBER: 1949:10919 CAPLUS
DOCUMENT NUMBER: 43:10919
ORIGINAL REFERENCE NO.: 43:2200d-1,2201a-e
TITLE: Derivatives of 3-hydroxythianaphthene
AUTHOR(S): Rodionov, V. M.; Bogoslovskii, B. M.; Kazakova, Z. S.
SOURCE: Izvestiya Akademii Nauk SSSR, Seriya Khimicheskaya (1948) 536-47
CODEN: IASKA6; ISSN: 0002-3353
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
G1 For diagram(s), see printed CA Issue.
AB o-HSC6H4CO2H (I) (3 g.), 2 g. ClCH2Ac, and 6.6 g. crystalline NaOAc in 100 ml. EtOH, let stand 10 hrs., then diluted with 200 ml. H2O, acidified by HCl, and concentrated to 150 ml. give 80.7% 5-acetonylthiosalicylic acid, m. 153-4° (from EtOH); this is obtained also in 78% yield by heating to 100° 2 hrs. 7.6 g. (o-HO2CC6H4)2S (II), 6 g. ClCH2Ac, 10 ml. 40% NaOH, 20 ml. water, and 10 ml. EtOH. I (6 g.), 3.7 g. ClCH2Ac, and 6.5 g. dry NaOH in 100 ml. absolute EtOH heated 10 hrs. on a steam bath, concentrated to 0.5 volume, poured into ice water, and acidified by HCl, give 86% 2-acetyl-3-hydroxythianaphthene, m. 81° (from 40% EtOH), soluble in dilute NaOH. This (1 g.) heated with Ac2O gives 2,3-diacetyl-3-hydroxythianaphthene, yellow, m. 126° (from EtOH). I (3.2 g.), 3.2 g. BrCH2Cl, and 5.4 g. crystalline NaOAc let stand 6 hrs. in 100 ml. EtOH, followed by dilution with water, give 89% 2-BzCH2SC6H4CO2H, m. 182° (from 50% EtOH); similar reaction using 3.3 g. dry NaOAc at reflux for 20 hrs. gives 75% 2-benzoyl-3-hydroxythianaphthene, yellow, m. 118° (from EtOH), soluble in hot 5% NaOH; the 3-Ac derivative, made with Ac2O, m. 105° (from EtOH). II (7.6 g.) or 7.7 g. I in 20 ml. water and 10 ml. 40% NaOH, treated with 10 g. BrCH2CH(OMe)2 in 10 ml. EtOH, followed by 2 hrs. heating, cooling, and acidification by HCl on dilution, give 63% o-HO2CC6H4SCH2CH(OMe)2, m. 114-15° (from C6H6), which with a trace of warm dilute acids reverts to the aldehyde, o-HO2CC6H4SCH2CHO (III), m. 156°, best obtained (90%) by solution of 1.5 g. I, 2 g. BrCH2CH(OMe)2, and 2.6 g. crystalline NaOAc in 50 ml. EtOH and treatment with 150 ml. cold H2O and 3-4 ml. concentrated HCl, followed by 1 hr. on a steam bath and concentration; on crystallization from water it gives a dihydrate, m. 159°, while on treatment with NH3-AgO it gives o-HO2CC6H4SCH2CO2H, m. 213°. III gives the oxime, m. 152° (from 50% EtOH). III (0.8 g.) in 10 ml. EtOH and 0.15 g. N2H4.H2O, let stand 1.0 hr. and heated 0.5 hr., followed by cooling and dilution, give 54% azine derivative (o-HO2CC6H4SCH2CH=N)2, m. 147° (from 50% EtOH). III gives a semicarbazone, m. 185° (from 50% MeOH). III oxime (4.5 g.) heated with 30 ml. Ac2O 1 hr. to 100°, followed by heating with 0.75 g. P2O5 and treatment with water, gives the nitrile, o-HO2CC6H4SCH2CN, m. 195-8° (from AcOH, then PhMe); use of SOCl2 in this preparation gives a cyanine dye, which can be prepared in 90% yield by heating 3-hydroxythianaphthene to 100° with 100% HCO2H; the red product, CO.C6H4.S.CHCH.C5.C6H4.CO, decompose 270° (from EtOH). III (1 g.), 0.9 g. hippuric acid, and 1.6 g. dry NaOAc with 20 ml. Ac2O heated 0.5 hr. give 88.7% of the oxazolone, o-HO2CC6H4SCH2CH:C.N:CPh.O.CO, m. 230° (from AcOH), on cooling and dilution with EtOH. III (2 g.) boiled 10 min. with 15 ml. Ac2O, then poured on ice, gives 62% 2-formyl-3-hydroxythianaphthene, yellowish, m. 107° (from 30% EtOH), which gives the Ag mirror test only in the absence of NaOH; the latter (1.8 g.) in 50% AcOH treated with 1 g. N2H4.H2O gives 66% azine derivative, [S.C6H4.C(OH).CCH=N]2, yellow, m.

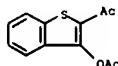
L3 ANSWER 13 OF 14 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
 198° (from C6H6); use of EtOH solvent always gives the cyanine dye described above. The formyl deriv. yields a semicarbazone, m. 185° (from 20% EtOH).
 IT 27468-08-2P, Ketone, 3-hydroxy-2-thianaphthenyl methyl, acetate
 97457-72-2P, Ketone, 3-hydroxy-2-thianaphthenyl phenyl, acetate
 RL: PREP (Preparation)
 RN (preparation of)
 27468-08-2 CAPLUS
 CN Ketone, 3-hydroxybenzo[b]thien-2-yl methyl, acetate (8CI) (CA INDEX NAME)



RN 97457-72-2 CAPLUS
 CN Methanone, [3-(acetyloxy)benzo[b]thien-2-yl]phenyl- (9CI) (CA INDEX NAME)



L3 ANSWER 14 OF 14 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1941:30357 CAPLUS
 DOCUMENT NUMBER: 35:30357
 ORIGINAL REFERENCE NO.: 35:4769g-1,4770a
 TITLE: Dismutation of some disulfides. IV
 AUTHOR(S): Fowkes, F. S.; McClelland, E. W.
 SOURCE: Journal of the Chemical Society (1941) 187-90
 CODEN: JCSOA9; ISSN: 0368-1769
 DOCUMENT TYPE: Journal
 LANGUAGE: Unavailable
 AB cf. C. A. 28, 5439.9. It is shown that Cl in the p-position to S decreases the tendency of a 2,2'-bithiobenzoic acid (I) to undergo dismutation. In consequence the 5,5'-di-Cl derivative (II) of I reacts less readily than I with Ac2CH2 in H2SO4 but yields similar products. II (1 g.), 1.25 g. AcOK and 12 cc. Ac2O, heated 4 hrs. at 130° (little reaction at 125° in 2 hrs.) and the product distilled with steam at 100°, give 0.05 g. 5-chloro-3-hydroxy-2-acetyl-1-thianaphthene (III), yellow, m. 166°, and 0.2 g. of 5-chloro-3-acetoxy-1-thianaphthene (IV), m. 67°. Reaction of 0.56 g. Ac2CH2 (added during 1 hr.) with 1 g. II in 8 cc. concentrated H2SO4 for 40 min. at 50-5° gives 0.75 g. III; it gives an olive-green color with FeCl3 in EtOH. Refluxing III with Ac2O in PhMe containing a trace of C5H5N for 6 hrs. gives the 3-Ac derivative, m. 132°, 3-acetoxy-2-acetyl-1-thianaphthene, m. 127°. Refluxing 1 g. III and 1.45 g. PhNHNH2 in C6H6 for 3 hrs. gives the hydrazone, yellow, m. 162°; boiling in EtOH containing 1 drop of concentrated H2SO4 for 30 min. gives 8-chloro-1-phenyl-3-methyl-4,5-thianaphthenopyrazole, m. 135°. III with H2O2 in AcOH (3 days at room temperature) gives the 1,1-dioxide, m. 265°. 5-Chloro-3-hydroxy-1-thianaphthene and PhNHNH2 in AcOH, heated at 100° for 35 min., give 10-chlorothianaphthindole, m. 222°; IV gives the same product; isatin in H2SO4 gives a blue color. H2O2 in AcOH transforms IV (4.5 days, with frequent shaking) into the 1,1-dioxide, m. 164°; if the reaction is heated at 100° for 1 hr. there results 5-chloro-3-hydroxy-1-thianaphthene 1,1-dioxide, m. 194°; the hydrazone, yellow, m. 290-2°, could not be indolized. Refluxing 30 g. I in 1 l. xylene with 20 g. P255 for 6 hrs. gives 75% of 2,3-dithiosulfindene; this reaction suggests that I undergoes dismutation in neutral as well as in acid media.
 IT 27468-08-2P, Ketone, 3-hydroxy-2-thianaphthenyl methyl, acetate
 RL: PREP (Preparation)
 RN (preparation of)
 27468-08-2 CAPLUS
 CN Ketone, 3-hydroxybenzo[b]thien-2-yl methyl, acetate (8CI) (CA INDEX NAME)



chain nodes :
 10 11 12 13 14 16 17 18 20 21 22 27
 ring nodes :
 1 2 3 4 5 6 7 8 9
 chain bonds :
 7-13 8-10 10-11 10-12 13-14 14-27 16-17 16-20 17-18 21-22
 ring bonds :
 1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9
 exact/norm bonds :
 5-7 6-9 7-8 7-13 8-9 10-11 10-12 13-14 14-27 16-17 16-20 17-18 21-22
 exact bonds :
 8-10
 normalized bonds :
 1-2 1-6 2-3 3-4 4-5 5-6

G1:Cb,Ak

G2:H,Cb,Cy,Ak

G3:[*1],[*2]

Match level :
 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS
 11:CLASS 12:CLASS 13:CLASS 14:CLASS 16:CLASS 17:CLASS 18:CLASS 20:CLASS
 21:CLASS 22:CLASS 27:CLASS

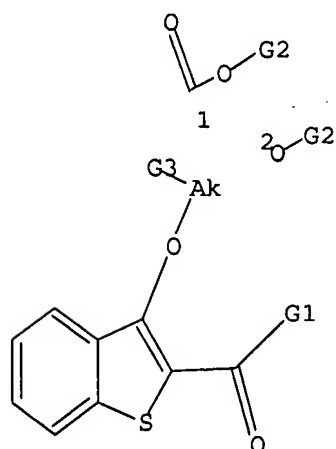
L4 STRUCTURE UPLOADED

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L4 HAS NO ANSWERS

L4 STR

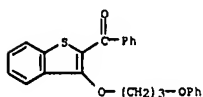


G1 Cb,Ak

G2 H,Cb,Cy,Ak

G3 [@1],[@2]

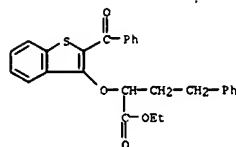
L5 ANSWER 1 OF 10 REGISTRY COPYRIGHT 2007 ACS on STN
 RN 852430-19-4 REGISTRY
 ED Entered STN: 16 Jun 2005
 CN Methanone, [3-(3-phenoxypropoxy)benzo[b]thien-2-yl]phenyl- (9CI) (CA INDEX NAME)
 OTHER NAMES:
 CN [3-(3-Phenoxypropoxy)benzo[b]thiophen-2-yl]phenylmethanone
 MF C24 H20 O3 S
 SR CA
 LC STN Files: CA, CAPLUS, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

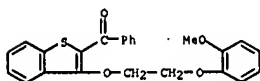
L5 ANSWER 2 OF 10 REGISTRY COPYRIGHT 2007 ACS on STN
 RN 852430-18-3 REGISTRY
 ED Entered STN: 16 Jun 2005
 CN Benzenebutanoic acid, α-[(2-benzoylbenzo[b]thien-3-yl)oxy]-, ethyl ester (9CI) (CA INDEX NAME)
 OTHER NAMES:
 CN Ethyl 2-[(2-benzoylbenzo[b]thiophen-3-yl)oxy]-4-phenylbutyrate
 MF C27 H24 O4 S
 SR CA
 LC STN Files: CA, CAPLUS, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

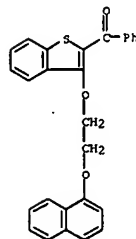
L5 ANSWER 3 OF 10 REGISTRY COPYRIGHT 2007 ACS on STN
 RN 852430-16-1 REGISTRY
 ED Entered STN: 16 Jun 2005
 CN Methanone, [3-[2-(2-methoxyphenoxy)ethoxy]benzo[b]thien-2-yl]phenyl- (9CI) (CA INDEX NAME)
 OTHER NAMES:
 CN [3-[2-(2-Methoxyphenoxy)ethoxy]benzo[b]thiophen-2-yl]phenylmethanone
 MF C24 H20 O4 S
 SR CA
 LC STN Files: CA, CAPLUS, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

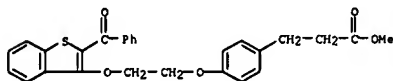
L5 ANSWER 4 OF 10 REGISTRY COPYRIGHT 2007 ACS on STN
 RN 852430-15-0 REGISTRY
 ED Entered STN: 16 Jun 2005
 CN Methanone, [3-[2-(1-naphthalenyloxy)ethoxy]benzo[b]thien-2-yl]phenyl- (9CI) (CA INDEX NAME)
 OTHER NAMES:
 CN [3-[2-(Naphthalen-1-yloxy)ethoxy]benzo[b]thiophen-2-yl]phenylmethanone
 MF C27 H20 O3 S
 SR CA
 LC STN Files: CA, CAPLUS, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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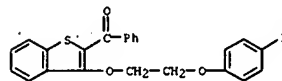
L5 ANSWER 5 OF 10 REGISTRY COPYRIGHT 2007 ACS on STN
 RN 852430-14-9 REGISTRY
 ED Entered STN: 16 Jun 2005
 CN Benzenepropanoic acid, 4-[2-[(2-benzoylbenzo[b]thien-3-yl)oxy]ethoxy]-, methyl ester (9C1) (CA INDEX NAME)
 OTHER NAMES:
 CN Methyl 3-[4-[2-[(2-Benzoylbenzothiophen-3-yl)oxy]ethoxy]phenyl]propionate
 MF C27 H24 O5 S
 SR CA
 LC STN Files: CA, CAPLUS, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

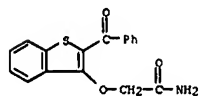
L5 ANSWER 6 OF 10 REGISTRY COPYRIGHT 2007 ACS on STN
 RN 852430-12-7 REGISTRY
 ED Entered STN: 16 Jun 2005
 CN Methanone, [3-[2-(4-fluorophenoxy)ethoxy]benzo[b]thien-2-yl]phenyl- (9C1) (CA INDEX NAME)
 OTHER NAMES:
 CN [3-[2-(4-Fluorophenoxy)ethoxy]benzo[b]thiophen-2-yl]phenylmethanone
 MF C23 H17 F O3 S
 SR CA
 LC STN Files: CA, CAPLUS, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

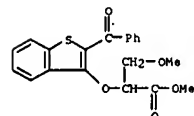
L5 ANSWER 7 OF 10 REGISTRY COPYRIGHT 2007 ACS on STN
 RN 852430-11-6 REGISTRY
 ED Entered STN: 16 Jun 2005
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 OTHER NAMES:
 CN 2-[(2-Benzoylbenzothiophen-3-yl)oxy]acetamide
 MF C17 H13 N O3 S
 SR CA
 LC STN Files: CA, CAPLUS, USPATFULL



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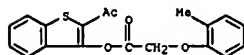
L5 ANSWER 8 OF 10 REGISTRY COPYRIGHT 2007 ACS on STN
 RN 852430-00-3 REGISTRY
 ED Entered STN: 16 Jun 2005
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 OTHER NAMES:
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 MF C20 H18 O5 S
 SR CA
 LC STN Files: CA, CAPLUS, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

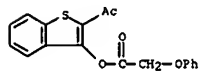
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 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L5 ANSWER 9 OF 10 REGISTRY COPYRIGHT 2007 ACS on STN
 RN 372977-92-9 REGISTRY
 ED Entered STN: 03 Dec 2001
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 (CA INDEX NAME)
 MF C19 H16 O4 S
 SR Chemical Library
 Supplier: Interbioscreen Ltd.
 LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 ANSWER 10 OF 10 REGISTRY COPYRIGHT 2007 ACS on STN
 RN 372972-28-6 REGISTRY
 ED Entered STN: 03 Dec 2001
 CN Acetic acid, phenoxy-, 2-acetylbenzo[b]thien-3-yl ester (9CI) (CA INDEX
 NAME)
 MF C18 H14 O4 S
 SR Chemical Library
 Supplier: Interbioscreen Ltd.
 LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
191.60	435.25

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
0.00	-11.70

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FILE LAST UPDATED: 13 Jul 2007 (20070713/ED)

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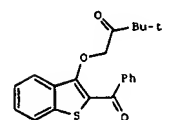
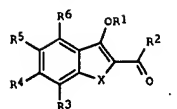
<http://www.cas.org/infopolicy.html>

=> s 15
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ACCESSION NUMBER: 2005:45342 CAPLUS
 DOCUMENT NUMBER: 143:7588
 TITLE: Preparation of benzofuran and benzothiophene derivatives as antidiabetic agents
 INVENTOR(S): Moineau, Gerard; Leriche, Caroline; Kergoat, Micheline
 PATENT ASSIGNER(S): Merck Santé, Fr.
 SOURCE: Fr. Demande, 55 pp.
 CODEN: FRXXBL
 DOCUMENT TYPE: Patent
 LANGUAGE: French
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2862646	A1	20050527	FR 2003-13615	20031120
FR 2862646	B1	20060224		
AU 2004295036	A1	20050616	AU 2004-295036	20041108
CA 2546651	A1	20050616	CA 2004-2546651	20041108
WO 2005054226	A1	20050616	WO 2004-EP12620	20041108
W: AR, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GR, GU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TH, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZH, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1685122	A1	20060802	EP 2004-797711	20041108
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK, IS				
CN 1882562	A	20061220	CN 2004-80034191	20041108
BR 2004016790	A	20070306	BR 2004-16790	20041108
JP 2007511556	T	20070510	JP 2006-540238	20041108
IN 2006KN00984	A	20070420	IN 2006-KN984	20060419
US 2007066680	A1	20070322	US 2006-579996	20060519
PRIORITY APPLN. INFO:			FR 2003-13615	A 20031120
OTHER SOURCE(S):			WO 2004-EP12620	W 20041108
GI			CASREACT 143:7588; MARPAT 143:7588	



AB Title compds. I [wherein X = O, S; R1 = carbonylalkyl, alkoxyalkyl, arylalkoxyalkyl, etc.; R2 = cycloalkyl, aryl; R3, R4, R5, R6 = independently H, halo, OH, alkyl, alkoxy, CN, CF3, NO2, NH2 and derivs.; their stereoisomers, racemates and pharmaceutically acceptable salts] were prepared as antidiabetic agents for treat diseases associated with insulin resistance syndrome. For example, II was prepared by cyclocondensation of thiosalicylic acid with 2-bromoacetophenone, followed by reaction with 1-bromopinacolone. In an in vitro test, at 10⁻⁶ M, II displayed a glucose-induced stimulation factor of insulin secretion of 183% at a dose of 8 mM glucose digested by the pancreatic exocrine tissue of rats. II, when administered orally to NOSTZ rats, reduced glycemia level by 23%. Thus, and their compns. are used for treating hyperglycemia, diabetes, dyslipidemia, obesity, and microvascular and macrovascular complications arising from diabetes.

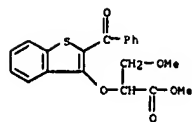
IT 852430-00-3P, 2-[(2-Benzoylbenzothiophen-3-yl)oxy]-3-methoxypropionic acid methyl ester 852430-11-6P, 2-[(2-Benzoylbenzothiophen-3-yl)oxy]acetamide 852430-12-7P, [3-(2-(4-Fluorophenoxy)ethoxy)benzo[b]thiophen-2-yl]phenylmethanone 852430-14-9P, Methyl 3-[4-[(2-Benzoylbenzothiophen-3-yl)oxy]ethoxy]phenylpropionate 852430-15-0P, [3-(2-(Naphthalen-1-yl)oxy)ethoxy]benzo[b]thiophen-2-yl]phenylmethanone 852430-16-1P, [3-(2-(2-Methoxyphenoxy)ethoxy)benzo[b]thiophen-2-yl]phenylmethanone 852430-18-3P, Ethyl 2-[(2-Benzoylbenzothiophen-3-yl)oxy]-4-phenylbutyrate 852430-19-4P, [3-(3-Phenoxypropoxy)benzo[b]thiophen-2-yl]phenylmethanone

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

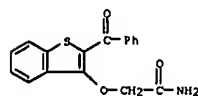
(drug candidate; preparation of benzofuran and benzothiophene derivs. as antidiabetic agents)

RN 852430-00-3 CAPLUS

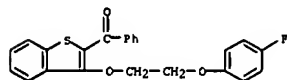
CN Propanoic acid, 2-[(2-benzoylbenzo[b]thien-3-yl)oxy]-3-methoxy-, methyl ester (9CI) (CA INDEX NAME)



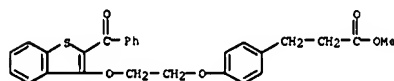
RN 852430-11-6 CAPLUS
 CN Acetamide, 2-[(2-benzoylbenzo[b]thien-3-yl)oxy]- (9CI) (CA INDEX NAME)



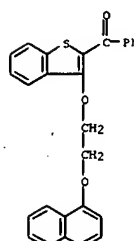
RN 852430-12-7 CAPLUS
 CN Methanone, [3-(2-(4-fluorophenoxy)ethoxy)benzo[b]thien-2-yl]phenyl- (9CI) (CA INDEX NAME)



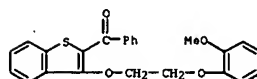
RN 852430-14-9 CAPLUS
 CN Benzenepropanoic acid, 4-[2-[(2-benzoylbenzo[b]thien-3-yl)oxy]ethoxy]-, methyl ester (9CI) (CA INDEX NAME)



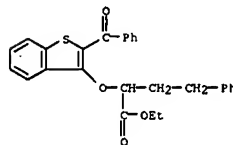
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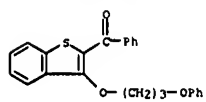
RN 852430-16-1 CAPLUS
 CN Methanone, [3-(2-(2-methoxyphenoxy)ethoxy)benzo[b]thien-2-yl]phenyl- (9CI) (CA INDEX NAME)



RN 852430-18-3 CAPLUS
 CN Benzenebutanoic acid, α-[(2-benzoylbenzo[b]thien-3-yl)oxy]-, ethyl ester (9CI) (CA INDEX NAME)



RN 852430-19-4 CAPLUS
 CN Methanone, [3-(3-phenoxypropoxy)benzo[b]thien-2-yl]phenyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

7-13 8-10 10-11 10-12 13-14 14-27 16-17 16-20 17-18 21-22
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 1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9
 exact/norm bonds :
 5-7 6-9 7-8 7-13 8-9 10-11 10-12 13-14 14-27 16-17 16-20 17-18 21-22
 exact bonds :
 8-10
 normalized bonds :
 1-2 1-6 2-3 3-4 4-5 5-6

G1:Cb,Ak

G2:H,Cb,Cy,Ak,Hy

G3:[*1],[*2]

Match level :

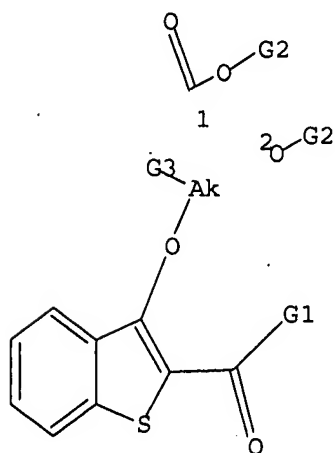
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 11:CLASS 12:CLASS 13:CLASS 14:CLASS 16:CLASS 17:CLASS 18:CLASS 20:CLASS
 21:CLASS 22:CLASS 27:CLASS

L1 STRUCTURE UPLOADED

=> d

L1 HAS NO ANSWERS

L1 STR



G1 Cb,Ak

G2 H,Cb,Cy,Ak,Hy

G3 [@1],[@2]

Structure attributes must be viewed using STN Express query preparation.

=> s l1 full

FULL SEARCH INITIATED 15:28:15 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 2917 TO ITERATE

100.0% PROCESSED 2917 ITERATIONS

10 ANSWERS

SEARCH TIME: 00.00.01

L2 10 SEA SSS FUL L1

=> d 12 11-10
'11-10' IS NOT A VALID FORMAT FOR FILE 'REGISTRY'

The following are valid formats:

Substance information can be displayed by requesting individual fields or predefined formats. The predefined substance formats are: (RN = CAS Registry Number)

REG - RN
SAM - Index Name, MF, and structure - no RN
FIDE - All substance data, except sequence data
IDE - FIDE, but only 50 names
SQIDE - IDE, plus sequence data
SQIDE3 - Same as SQIDE, but 3-letter amino acid codes are used
SQD - Protein sequence data, includes RN
SQD3 - Same as SQD, but 3-letter amino acid codes are used
SQN - Protein sequence name information, includes RN

CALC - Table of calculated properties
EPROP - Table of experimental properties
PROP - EPROP and CALC

Any CA File format may be combined with any substance format to obtain CA references citing the substance. The substance formats must be cited first. The CA File predefined formats are:

ABS -- Abstract
APPS -- Application and Priority Information
BIB -- CA Accession Number, plus Bibliographic Data
CAN -- CA Accession Number
CBIB -- CA Accession Number, plus Bibliographic Data (compressed)
IND -- Index Data
IPC -- International Patent Classification
PATS -- PI, SO
STD -- BIB, IPC, and NCL

IABS -- ABS, indented, with text labels
IBIB -- BIB, indented, with text labels
ISTD -- STD format, indented

OBIB ----- AN, plus Bibliographic Data (original)
OIBIB ----- OBIB, indented with text labels

SBIB ----- BIB, no citations
SIBIB ----- IBIB, no citations

The ALL format gives FIDE BIB ABS IND RE, plus sequence data when it is available.

The MAX format is the same as ALL.

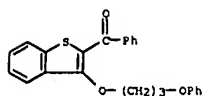
The IALL format is the same as ALL with BIB ABS and IND indented, with text labels.

For additional information, please consult the following help messages:

HELP DFIELDS -- To see a complete list of individual display fields.
HELP FORMATS -- To see detailed descriptions of the predefined formats.
ENTER DISPLAY FORMAT (IDE):end

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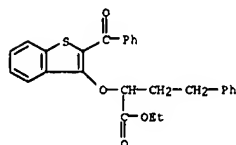
L2 ANSWER 1 OF 10 REGISTRY COPYRIGHT 2007 ACS on STN
 RN 852430-19-4 REGISTRY
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 CN Methanone, [3-(3-phenoxypropoxy)benzo[b]thien-2-yl]phenyl- (9CI) (CA INDEX NAME)
 OTHER NAMES:
 CN [3-(3-phenoxypropoxy)benzo[b]thiophen-2-yl]phenylmethanone
 MF C24 H20 O3 S
 SR CA
 LC STN Files: CA, CAPLUS, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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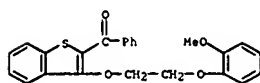
L2 ANSWER 2 OF 10 REGISTRY COPYRIGHT 2007 ACS on STN
 RN 852430-18-3 REGISTRY
 ED Entered STN: 16 Jun 2005
 CN Benzenebutanoic acid, α-[(2-benzoylbenzo[b]thien-3-yl)oxy]-, ethyl ester (9CI) (CA INDEX NAME)
 OTHER NAMES:
 CN Ethyl 2-[(2-benzoylbenzo[b]thiophen-3-yl)oxy]-4-phenylbutyrate
 MF C27 H24 O4 S
 SR CA
 LC STN Files: CA, CAPLUS, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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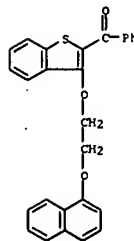
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 OTHER NAMES:
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 MF C24 H20 O4 S
 SR CA
 LC STN Files: CA, CAPLUS, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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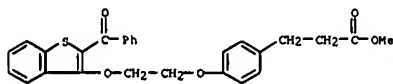
L2 ANSWER 4 OF 10 REGISTRY COPYRIGHT 2007 ACS on STN
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 OTHER NAMES:
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 MF C27 H20 O3 S
 SR CA
 LC STN Files: CA, CAPLUS, USPATFULL



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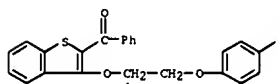
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 OTHER NAMES:
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 MF C27 H24 O5 S
 SR CA
 LC STN Files: CA, CAPLUS, USPATFULL



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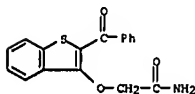
L2 ANSWER 6 OF 10 REGISTRY COPYRIGHT 2007 ACS on STN
 RN 852430-12-7 REGISTRY
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 OTHER NAMES:
 CN [3-[2-(4-Fluorophenoxy)ethoxy]benzo[b]thiophen-2-yl]phenylmethanone
 MF C23 H17 F O3 S
 SR CA
 LC STN Files: CA, CAPLUS, USPATFULL



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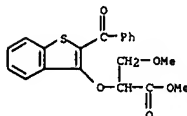
L2 ANSWER 7 OF 10 REGISTRY COPYRIGHT 2007 ACS on STN
 RN 852430-11-6 REGISTRY
 ED Entered STN: 16 Jun 2005
 CN Acetamide, 2-[(2-benzoylbenzo[b]thien-3-yl)oxy]- (9CI) (CA INDEX NAME)
 OTHER NAMES:
 CN 2-[(2-Benzoylbenzothiophen-3-yl)oxy]acetamide
 MF C17 H13 N O3 S
 SR CA
 LC STN Files: CA, CAPLUS, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

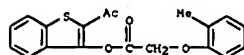
L2 ANSWER 8 OF 10 REGISTRY COPYRIGHT 2007 ACS on STN
 RN 852430-00-3 REGISTRY
 ED Entered STN: 16 Jun 2005
 CN Propanoic acid, 2-[(2-benzoylbenzo[b]thien-3-yl)oxy]-3-methoxy-, methyl ester (9CI) (CA INDEX NAME)
 OTHER NAMES:
 CN 2-[(2-Benzoylbenzothiophen-3-yl)oxy]-3-methoxypropionic acid methyl ester
 MF C20 H18 O5 S
 SR CA
 LC STN Files: CA, CAPLUS, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

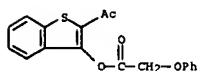
1 REFERENCES IN FILE CA (1907 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L2 ANSWER 9 OF 10 REGISTRY COPYRIGHT 2007 ACS on STN
 RN 372977-92-9 REGISTRY
 ED Entered STN: 03 Dec 2001
 CN Acetic acid, (2-methylphenoxy)-, 2-acetylbenzo[b]thien-3-yl ester (9CI)
 (CA INDEX NAME)
 MF C19 H16 O4 S
 SR Chemical Library
 Supplier: Interbioscreen Ltd.
 LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 ANSWER 10 OF 10 REGISTRY COPYRIGHT 2007 ACS on STN
 RN 372972-28-6 REGISTRY
 ED Entered STN: 03 Dec 2001
 CN Acetic acid, phenoxy-, 2-acetylbenzo[b]thien-3-yl ester (9CI) (CA INDEX NAME)
 MF C18 H14 O4 S
 SR Chemical Library
 Supplier: Interbioscreen Ltd.
 LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

LJ ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN
 AN 2005:453342 CAPLUS
 DN 143:7588
 TI Preparation of benzofuran and benzothiophene derivatives as antidiabetic agents
 IN Moinet, Gerard; Leriche, Caroline; Kergoat, Micheline
 PA Merck Santa, Fr.
 SO Fr. Demande, 55 pp.
 CODEN: FRXXBL
 DT Patent
 LA French
 FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2862646	A1	20050527	FR 2003-13615	20031120
FR 2862646	B1	20060224		
AU 2004295036	A1	20050616	AU 2004-295036	20041108
CA 2546651	A1	20050616	CA 2004-2546651	20041108
WO 2005054226	A1	20050616	WO 2004-EP12620	20041108
WI AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BV, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, ME, MK, MN, MW, MX, MY, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GN, GQ, GW, ML, HR, NE, SN, TD, TG				
EP 1685122	A1	20060802	EP 2004-797711	20041108
RI AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK, IS				
CN 1882562	A	20061220	CN 2004-80034191	20041108
BR 2004016790	A	20070306	BR 2004-16790	20041108
JP 2007511556	T	20070510	JP 2006-540238	20041108
IN 2006000984	A	20070420	IN 2006-KN984	20060419
US 2007066680	A1	20070322	US 2006-579996	20060519
PRAI FR 2003-13615	A	20031120		
WO 2004-EP12620	W	20041108		
OS CASREACT 143:7588; HARPAT 143:7588				
RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD				
ALL CITATIONS AVAILABLE IN THE RE FORMAT				